

**THERMAL:
A Routine Designed to Calculate Neutron
Thermal Scattering**

by
Dermott E. Cullen
Lawrence Livermore National Laboratory
L-294
P.O. Box 808
Livermore, CA 94550

September 19, 1995

**THERMAL:
A Routine Designed to Calculate Neutron
Thermal Scattering**

by
Dermott E. Cullen
Lawrence Livermore National Laboratory
L-294
P.O. Box 808
Livermore, CA 94550

September 19, 1995

Introduction

THERMAL is designed to calculate neutron thermal scattering that is elastic and isotropic in the center of mass system. At low energy thermal motion will be included. At high energies the target nuclei are assumed to be stationary. The point of transition between low and high energies has been defined to insure a smooth transition.

It is assumed that at low energy the elastic cross section is constant in the relative system. At high energy the cross section can be of any form.

You can use this routine for all energies where the elastic scattering is isotropic in the center of mass system. In most materials this will be a fairly high energy, e.g., the keV energy range.

The THERMAL method is simple, clean, easy to understand, and most important very efficient; on a IBM-PC Pentium Pro 200, at low energies with thermal scattering it can do about 9 million scatters a minute and at high energy about 31 million.

Warning: This version of THERMAL completely supersedes the original version described in the same report number, dated February 24, 1995. The method used in the original code is **incorrect**, as explained in this report.

Documentation

This routine is designed to be self-documenting, in the sense that the latest documentation for the routine is included as comment lines at the beginning of the routine. Reports, such as this one, are periodically published. However, the user should be aware that the comment lines within the routine are continuously updated to reflect the most recent status of the routine and these comment lines must always be considered the most recent

documentation. Therefore the user is advised to always read the comment lines within the routine.

Acknowledgments

I thank Gene Canfield, (Lawrence Livermore National Laboratory) for contributing his time, energy and most of all his ideas concerning thermal scattering. I also thank Jim Rathkopf, (Lawrence Livermore National Laboratory) and Ray Tolar, (University of Michigan) for contributing their ideas.

Background

THERMAL is designed to calculate neutron thermal scattering that is elastic and isotropic in the center of mass system. At low energy thermal motion will be included. At high energies the target nuclei are assumed to be stationary. The point of transition between low and high energies has been defined to insure a smooth transition.

It is assumed that at low energy the elastic cross section is constant in the relative system. At high energy the cross section can be of any form.

You can use this routine for all energies where the elastic scattering is isotropic in the center of mass system. In most materials this will be a fairly high energy, e.g., the keV energy range.

The THERMAL method is simple, clean, easy to understand, and most important very efficient; on an IBM-PC Pentium Pro 200, at low energies with thermal scattering it can do about 9 million scatters a minute and at high energy about 31 million.

Warning: This version of THERMAL completely supersedes the original version described in the same report number, dated February 24, 1995. The method used in the original code is **incorrect**, as explained in this report.

Before introducing the THERMAL model I will first cover the background information needed to understand thermal scattering. In particular I will try to describe all assumptions and approximations used, so that the reader can clearly understand the range of validity of the method.

How to do Thermal Scattering

It is recommended that for those materials that thermal scattering law data is available you use it; this will give you the best representation of thermal scattering. However, thermal scattering law data is only available for a few materials, whereas typical nuclear data files contain data for a hundred or more materials. THERMAL is designed to be used for those materials that thermal scattering law data is not available, i.e., most of the materials in nuclear data files. It is recommended that the "high" energy THERMAL treatment be used for all materials for all energies above thermal up to the highest energy where the elastic scattering is still isotropic in the center of mass system. Do not fail to appreciate the advantage of using this higher energy treatment; it is very efficient and fast,

on an IBM PC Pentium Pro 200 being able to process about 31million scatters per minute.

Frame of Reference

In this report I will use three frames of reference,

The **Lab** frame of reference is a stationary frame of reference with regard to the bulk of the media through which the neutrons are transporting = my Lab. It is the system that we use to transport neutrons between spatial points during a transport calculation, i.e., we transport neutrons a given distance with reference to the media that it is passing through. Later when we discuss the distribution of target nuclei we will see that it is also the only system in which it makes sense to assume the targets are moving isotropically.

The **Relative** frame of reference is centered on and moving with the neutron. It is the system in which we can observe and define the actual neutron reaction rate, i.e., it is relative motion between neutron and target that leads to and defines the reaction rate. For each interaction there are two "particles", a neutron and a target, and in principle we could define the relative frame as centered on and moving with either. However, in selecting which interaction occurs we will consider one neutron and a known ensemble of target nuclei that the neutron could possibly interact with. Therefore it makes more sense to define the relative frame as centered on and moving with the one neutron.

The **Center of Mass** frame of reference is centered on and moving with the neutron+target mass. It is the system in which we will define the angular distribution of scattered neutrons and in which we will describe the actual kinematics of neutron scatter.

In the following discussion I will attempt to always clearly identify the frame or frames of reference. However, I will admit that the terminology sometimes becomes confusing, particularly with regard to Relative vs. Center of Mass frames. For example, it is fairly common practice when discussing the Doppler broadening equation to say that this equation conserves reactions in the Lab and Center of Mass system, whereas the only two systems explicitly involved are the Lab and Relative frames. I will try to make clear what systems I am using; my apologies in advance if I do not always succeed in making this clear.

Calculation of Reaction Rate

In normal temperature ranges the actual relative frame nuclear cross sections are not temperature dependent. The Doppler broadened cross section is temperature dependent because we need to perform calculations in the Lab frame of reference. The "apparent" temperature dependence is only due to the transformation between relative and Lab frames of reference. In this transformation we wish to conserve a physical observable: namely, the reaction rate in both systems.

The reaction rate is defined by the Doppler broadening equation, which conserves reaction rate in the relative and laboratory systems by defining the Doppler broadened (laboratory) cross section, $\text{sig}(v)$,

$$v \text{ sig}(v) = \langle v_r \text{ sig}(v_r) P(v_t) \rangle$$

Lab reactions = Relative reactions

v = laboratory speed

$\text{sig}(v)$ = Doppler broadened (laboratory) cross section

v_r = relative speed (relative between target nucleus and neutron)

$\text{sig}(v_r)$ = cross section at relative speed

$P(v_t)$ = distribution of target nuclei

One important point to understand: the cross sections in the relative frame of reference, $\text{sig}(v_r)$, are the so called "cold" cross sections that have not been Doppler broadened, and the speed, v_r , or equivalently the energy, E_r , are defined at relative speed and energy, not center of mass speed and energy, or in any other frame of reference. Starting from evaluated neutron data as it appears in most evaluated data files, such as ENDF/B, the data is "cold", where cross sections and resonances parameters are given at Lab neutron energies. "Cold" means that the medium is at zero Kelvin temperature, so that neutron Lab and relative speed and energy are equal. Therefore the "cold" data to use in the Doppler broadening equation is exactly the data as it appears in most evaluated data files, and to define the cross section in the Doppler broadening equation the relative speed or energy is the Lab speed or energy at which the "cold" data is tabulated. In particular, do not make the mistake of trying to use center of mass energies, or energy in any other frame of reference: just use the cross sections at exactly the energies at which they are tabulated.

From the units of v_r (cm/second), $\text{sig}(v_r)$ (1/cm), and $P(v_t) dv_t$ (dimensionless), the units of reactions $v \text{ sig}(v)$ or $\langle v_r \text{ sig}(v_r) P(v_t) \rangle$ is **1/seconds = reactions per second**.

Note, based on the units of the results, **1/seconds**, this equation **MUST NOT** be interpreted to define the **average relative speed**, which has units of cm/second; this point will be discussed in detail below.

Calculation of Average Relative Speed

The normalized distribution of relative speeds for targets that actually collide is defined by,

$$P = v_r \text{ sig}(v_r) P(v_t) / \langle v_r \text{ sig}(v_r) P(v_t) \rangle$$

and the average relative speed is defined by,

$$\begin{aligned}\langle v_r \rangle &= \langle v_r P \rangle / \langle P \rangle = \langle v_r P \rangle \\ &= \langle v_r^2 \text{sig}(v_r) P(v_t) \rangle / \langle v_r \text{sig}(v_r) P(v_t) \rangle\end{aligned}$$

The units of $\langle v_r \rangle$ are **cm/second**.

Note, based on the units of the results, **cm/second**, this equation **MUST NOT** be interpreted to define the **reaction rate**, which has units of **1/second**; this point will be discussed in detail below.

Consistent Reaction Rates: Part 1

In defining reaction rates we will consider the average time between collisions. The time between collisions is,

$$t = x / [v \text{sig}(v)]$$

where x is the distance to collision and is exponentially distributed and has an average expectation value of 1. In the following I will indicate this as $\langle 1 \rangle$.

From the Doppler broadening equation we have,

$$v \text{sig}(v) = \langle v_r \text{sig}(v_r) P(v_t) \rangle$$

so that the time between collisions is,

$$t = \langle 1 \rangle / [v \text{sig}(v)] = \langle 1 \rangle / \langle v_r \text{sig}(v_r) P(v_t) \rangle$$

The distribution of relative speeds is,

$$P = v_r \text{sig}(v_r) P(v_t) / \langle v_r \text{sig}(v_r) P(v_t) \rangle$$

In the LAB frame of reference,

$$\begin{aligned}\langle t \rangle &= \langle t P \rangle = \langle 1 \rangle [\langle v_r \text{sig}(v_r) P(v_t) \rangle / \langle v_r \text{sig}(v_r) P(v_t) \rangle] / \langle v_r \text{sig}(v_r) P(v_t) \rangle \\ &= \langle 1 \rangle / \langle v_r \text{sig}(v_r) P(v_t) \rangle\end{aligned}$$

In the Relative system we have,

$$t = \langle 1 \rangle / [v_r \text{sig}(v_r)]$$

$$\begin{aligned}\langle t \rangle &= \langle t P \rangle = \langle 1 \rangle [\langle v_r \text{sig}(v_r) P(v_t) / [v_r \text{sig}(v_r)] \rangle / \langle v_r \text{sig}(v_r) P(v_t) \rangle] \\ &= \langle 1 \rangle \langle P(v_t) \rangle / \langle v_r \text{sig}(v_r) P(v_t) \rangle \\ &= \langle 1 \rangle / \langle v_r \text{sig}(v_r) P(v_t) \rangle\end{aligned}$$

Therefore we have a consistent average time between events, and therefore a consistent reaction rate in the LAB and Relative systems.

This is an important result, since it means that in principle we can perform calculations in either the LAB or Relative system, and expect to obtain the same answer, at least as far as reaction rate. For example, in the Relative frame we can sample a relative speed, v_r , and cross section, $\text{sig}(v_r)$. These in turn can be used to define the distance and time to the next collision,

$$x = -\text{Log}(\text{random})/\text{sig}(v_r)$$

$$t = x/v_r = -\text{Log}(\text{random})/[v_r \text{ sig}(v_r)]$$

and at the collision site the relative speed, v_r , can be used to solve the kinematics equations to define the new neutron speed after the collision.

Alternatively, in the Lab system, we can define the distance and time to the next collision,

$$x = -\text{Log}(\text{random})/\text{sig}(v)$$

$$t = x/v = -\text{Log}(\text{random})/[v \text{ sig}(v)]$$

and at the collision site we can sample the relative speed, v_r , and use it to solve the kinematics equations to define the new neutron speed after the collision.

Whichever approach we use we expect the same reaction rate, since above we have seen that the expected average time between collision, $\langle t \rangle$, is the same in both systems,

$$\langle t \rangle = \langle 1 \rangle / \langle v_r \text{ sig}(v_r) \rangle = \langle 1 \rangle / [v \text{ sig}(v)]$$

Which Frame of Reference Should We Use?

As I said above, "in principle" we can use either frame of reference. In fact it is only practical to use the Lab frame of reference. From the above where we only considered average time between collisions, and therefore average reaction rate, we can use either system. However, there are some definite and practical reasons for only using the Lab frame,

1) In order to use the Relative frame we have to know the cross sections in the relative frame. This means we have to know the so called "cold" cross sections, that have not been Doppler broadened. In this report I will only be discussing the elastic cross section. But to actually perform transport calculations we need all of the cross sections. Trying to sample all cross sections to define the total in the relative frame is generally very difficult. But the real bottom line is that since the data in our application oriented nuclear data files have generally already been Doppler broadened to one or more temperatures, using the Relative frame is impractical.

2) If we consider the speed of convergence of average reaction rates the Lab frame has a definite advantage over the Relative frame. The reaction rate is,

Lab,

$$x = -\text{Log}(\text{random})/\text{sig}(v)$$

$$t = x/v = -\text{Log}(\text{random})/[v \text{ sig}(v)]$$

where $v \text{ sig}(v)$ has been pre-calculated from the Doppler broadening equation. Therefore the speed of convergence is based on the speed of convergence in sampling the exponentially distributed distance to collision.

Relative,

$$x = -\text{Log}(\text{random})/\text{sig}(v_r)$$

$$t = x/v_r = -\text{Log}(\text{random})/[v_r \text{ sig}(v_r)]$$

In this case we do not use the pre-calculated Doppler broadened results. Therefore the speed of convergence is based on the speed of convergence of not only the exponential distance to collision, but also on the speed of convergence of the distribution of $v_r \text{ sig}(v_r)$ to the Doppler broadened result $v \text{ sig}(v)$.

Therefore, in the Relative frame the speed of convergence of the reaction rate should be slower than in the Lab system.

3) Above we saw that the average time between collisions is the same in both systems. What about the average distance to collision?

In the Lab frame,

$$x = -\text{Log}(\text{random})/\text{sig}(v)$$

$$\langle x \rangle = \langle x P \rangle = \langle 1 \rangle \langle P/\text{sig}(v) \rangle$$

$$P = v_r \text{ sig}(v_r) P(v_t) / \langle v_r \text{ sig}(v_r) P(v_t) \rangle$$

$$\begin{aligned} \langle x \rangle &= \langle 1 \rangle \langle [v_r \text{ sig}(v_r) P(v_t) / \text{sig}(v)] \rangle / \langle v_r \text{ sig}(v_r) P(v_t) \rangle \\ &= \langle 1 \rangle \langle [v_r \text{ sig}(v_r) P(v_t)] \rangle / \langle v_r \text{ sig}(v_r) P(v_t) \rangle \text{sig}(v) \\ &= \langle 1 \rangle / \text{sig}(v) \end{aligned}$$

In the Lab frame the Doppler broadened cross section is used to define the distance to collision.

In the Relative frame,

$$x = -\text{Log}(\text{random})/\text{sig}(v_r)$$

$$\langle x \rangle = \langle x P \rangle = \langle 1 \rangle \langle P/\text{sig}(v_r) \rangle$$

$$P = v_r \text{sig}(v_r) P(v_t) / \langle v_r \text{sig}(v_r) P(v_t) \rangle$$

$$\begin{aligned} \langle x \rangle &= \langle 1' \rangle \langle [v_r \text{sig}(v_r) P(v_t) / \text{sig}(v_r)] \rangle / \langle v_r \text{sig}(v_r) P(v_t) \rangle \\ &= \langle 1' \rangle \langle v_r P(v_t) \rangle / \langle v_r \text{sig}(v_r) P(v_t) \rangle \\ &= \langle 1 \rangle \langle v_r P(v_t) \rangle / [v \text{sig}(v)] \end{aligned}$$

In general $\langle v_r P(v_t) \rangle$ is not a quantity that we explicitly conserve. Therefore the average distance to collision using Lab or Relative frame is not the same. If we consider the case of a constant relative cross section, $\text{sig}(v_r) = 1$, then,

$$\langle v_r \text{sig}(v_r) P(v_t) \rangle = \langle v_r P(v_t) \rangle = v \text{sig}(v)$$

and in the relative frame,

$$\langle x \rangle = \langle 1 \rangle$$

compared to the Lab frame solution,

$$\langle x \rangle = \langle 1 \rangle / \text{sig}(v)$$

In other words, if the relative frame is used the effect of the Doppler broadened cross section is ignored. Since at lower energies the Doppler broadened cross section will be larger than the constant "cold" cross section, ignoring the effect of Doppler broadening on the cross section will overestimate the distance to collision.

Bottom line: Only the Lab frame of reference is practical to use in applications.

Warning - there are a number of codes that actually use the relative frame: if they are using the relative frame speed and cross section to define the distance to collision as described above **what is being done is incorrect**. Consider the simplest case of a constant relative cross section where the macroscopic total cross section is 1 per cm, so that the mean free path is 1 cm. Since the cross section in the relative is constant, regardless of the relative speed selected the relative cross section will always be 1 per cm, and the mean free path 1 cm.

The relative frame cross section and mean free path cannot be used to transport neutrons in the Lab frame, because this would ignore the fact that a portion of the relative speed is not due to neutron motion in the Lab, but is rather due to target motion; note, there is a good reason that it is called the relative speed, and not the Lab speed. For example, in hydrogen at thermal energy the Lab (Doppler broadened) cross section is about 50 % higher than the "cold" relative cross section. This means that at this energy the motion of

the neutron contributes $2/3$ and the motion of the target $1/3$ to the relative speed. Therefore on average rather than the neutron moving 1 cm per collision in the Lab, the neutron is only moving $2/3$ cm per collision and the target moves $1/3$ cm per collision relative to the neutron, and the two speeds combine to yield a total relative distance of 1 cm per collision

If you want to consider the most extreme case, consider a stationary neutron. Due to thermal motion of the target nuclei the neutron will still interact and the sampled relative speed can be used to define the time between collisions. In this case how far did the neutron move between collision? Move? I said the neutron is stationary; it didn't move at all; all of the motion is due to target motion.

Per collision using the relative frame speed and cross section will conserve reaction rate, by conserving time between collisions, but this doesn't necessarily mean that it will conserve the overall time scale of a system. The reason is that by moving neutrons too far between collisions (based on the relative frame cross section), we are moving them further than they could have possibly moved, based on the average time between collisions, and over a number of collisions this can completely change the time scale of a system. Consider the case where we have neutrons at point A and we want to transport them to point B that is many, or at least a number of, mean free paths away from point A. If we use the relative frame cross section to predict the distance between collisions we will over predict the distance between collisions. The result will be that in transporting between point A and point B we will underestimate the number of collisions, and thereby overestimate the number of neutrons arriving at point B, and we will also cause the neutrons to arrive too early in time at point B.

Failure to consider this point ignores the effects of Doppler broadening and can lead to completely erroneous results. If you are using this approach and want to do it correctly, contact me.

Consistent Reaction Rates: Part 2

Now that we have decided to only use the Lab system, there are additional points to consider. In order to consistently use the Lab system we need Doppler broadened cross sections which: 1) have been Doppler broadened using a method that is consistent with the THERMAL method, 2) have been Doppler broadened to the temperature of the medium through which the neutrons are transporting.

The SIGMA1 method of Doppler broadening (see, ref. 1) is completely consistent with the THERMAL method and it is highly recommended that you use the SIGMA1 program (see ref. 2) to Doppler broaden your cross sections to any temperature, or temperatures, that you require for use in your applications; this handles point 1), discussed above.

The second point of insuring that the Doppler broadened cross sections that you use have been broaden to exactly the temperature of the medium, can present a problem to real applications involving different temperatures in different spatial zones, or even temperature gradients. There are a number of ways to solve this problem; the "best"

method to use is highly problem dependent. I'll not go into detail here, but if you have this problem contact me so that we can discuss your specific problem.

Constant Elastic Cross Section

Above I have considered the case of a general cross section. From this point on I will consider the specific case of the elastic cross section at low energy. In this case I will assume that the cross section in the relative frame, the so called "cold" cross section, that has not been Doppler broadened, is constant. For the case where $\sigma(v_r)$ is independent of v_r (or energy) the equations reduce to the simpler form,

Doppler Broadening Equation,

$$v \sigma(v) = \sigma \langle v_r P(v_t) \rangle$$

Average Relative Speed

$$\langle v_r \rangle = \langle v_r^2 P(v_t) \rangle / \langle v_r P(v_t) \rangle$$

The following will assume that $\sigma = 1$, so that all results for the Doppler broadening equation will be per barn of constant cross section. Since σ appears in both numerator and denominator of the definition of average relative speed, it cancels out and these results will be absolute.

Isotropic Target Distribution

We will assume that the distribution of target nuclei velocities is isotropic,

$$P(v_t) d(v_t) d(\mu) d(\phi) = P^*(v_t) d(v_t) d(\mu) d(\phi) / (4 \pi)$$

$\mu = \cos(\theta) = \text{angle relative to neutron's direction of motion}$
 $\phi = \text{azimuthal angle}$

Integrating over the azimuthal angle,

$$v \sigma(v) = \langle v_r P(v_t) \rangle = \langle d(\mu) \langle v_r P^*(v_t) d(v_t) \rangle \rangle / 2$$

Using,

$$v_r^2 = [v^2 - 2 \mu v v_t + v_t^2]$$

$$d(\mu) = v_r d(v_r) / [v v_t]$$

$$v \sigma(v) = \langle v_r P(v_t) \rangle = \langle v_r^2 d(v_r) \langle P^*(v_t) d(v_t) / v_t \rangle \rangle / [2 v]$$

where the integral over v_r is from zero to infinity, and the integral over v_t is from $|v - v_r|$ to $|v + v_r|$.

This is a general result for any isotropic distribution of target nuclei velocities.

Maxwellian Free Atom Model

We will assume that the distribution of target nuclei is isotropically distributed in a Maxwellian; the so called free atom model,

$$P^*(v_t) dv_t = (4/\pi)^{1/2} b^{3/2} v_t^2 \text{Exp}(-b v_t^2) dv_t$$

$$b = A/(2 k T)$$

$$A = \text{Ratio of atomic weight of target to atomic weight of neutron}$$

$$k = \text{Boltzmann's constant}$$

$$T = \text{Absolute temperature (Kelvin)}$$

$$v \text{ sig}(v) = \langle v_r P(v_t) \rangle = (2/\pi)^{1/2} \langle v_r^2 \int_0^\infty b^{3/2} v_t \text{Exp}(-b v_t^2) dv_t / v \rangle$$

$$2 \langle b^{1/2} v_t \text{Exp}(-b v_t^2) \rangle = \langle \text{Exp}(-b v_t^2) \rangle \langle b v_t^2 \rangle$$

$$v \text{ sig}(v) = \langle v_r P(v_t) \rangle = [(b/\pi)^{1/2}/v] \langle v_r^2 K(v, v_r) \rangle$$

$$K(v, v_r) = \text{Exp}[-b (v - v_r)^2] - \text{Exp}[-b (v + v_r)^2]$$

which is the normal form of the Doppler broadening equation that we are used to using.

$$v \text{ sig}(v) = \langle v_r P(v_t) \rangle = \langle K^*(v, v_r) \rangle$$

$$K^*(v, v_r) = (b/\pi)^{1/2} (v_r^2/v) \{ \text{Exp}[-b (v - v_r)^2] - \text{Exp}[-b (v + v_r)^2] \}$$

Note, in this equation v_r^2 comes from the change of integration variables from μ to v_r ; v_r , not v_r^2 , appears in the original equation.

Similarly the distribution of relative speeds can be written as,

$$\begin{aligned} P &= v_r P(v_t) / \langle v_r P(v_t) \rangle \\ &= K^*(v, v_r) dv_r / \langle K^*(v, v_r) \rangle \end{aligned}$$

and the average relative speed is,

$$\langle v_r \rangle = \langle v_r K^*(v, v_r) \rangle / \langle K^*(v, v_r) \rangle$$

Doppler Broadened Cross Section

For normalization we need the Doppler broadened cross section, or rather reaction rate,

$$v \text{ sig}(v) = \langle v_r P(v_t) \rangle = \langle K^*(v, v_r) d(v_r) \rangle$$

$$K^*(v, v_r) = (b/\pi)^{1/2} (v_r^2/v) \{ \text{Exp}[-b(v - v_r)^2] - \text{Exp}[-b(v + v_r)^2] \}$$

Changing variables,

$$\begin{aligned} y^2 &= b v^2 \\ x^2 &= b v_r^2 \end{aligned}$$

$$\text{sig}(y) = (1/\pi)^{1/2} / y^2 \langle x^2 \{ \text{Exp}[-(x - y)^2] - \text{Exp}[-(x + y)^2] \} d(x) \rangle$$

$$\text{sig}(y) = \text{sig}^*(y) - \text{sig}^*(-y)$$

$$\text{sig}^*(y) = (1/\pi)^{1/2} / y^2 \langle x^2 \text{Exp}[-(x - y)^2] d(x) \rangle$$

Changing variables,

$$\begin{aligned} Z &= x - y \\ x &= Z + y \\ d(x) &= d(Z) \end{aligned}$$

$$\text{sig}^*(y) = (1/\pi)^{1/2} / y^2 \langle (Z + y)^2 \text{Exp}[-Z^2] d(Z) \rangle$$

$$\text{sig}^*(y) = (1/\pi)^{1/2} / y^2 \text{Int}[-y \text{ to infinity}] (Z^2 + 2 y Z + y^2) \text{Exp}[-Z^2] d(Z)$$

$$\text{sig}^*(-y) = (1/\pi)^{1/2} / y^2 \text{Int}[+y \text{ to infinity}] (Z^2 - 2 y Z + y^2) \text{Exp}[-Z^2] d(Z)$$

Integrating and adding $\text{sig}^*(y)$ and $\text{sig}^*(-y)$,

$$y \text{ sig}(y) = [y + 1/(2 y)] \text{ERF}(y) + 1/(\pi)^{1/2} \text{Exp}(-y^2)$$

$$b^{1/2} v \text{ sig}(v) = [b^{1/2} v + 1/(2 b^{1/2} v)] \text{ERF}(b^{1/2} v) + 1/(\pi)^{1/2} \text{Exp}(-b v^2)$$

$$v \text{ sig}(v) = [v + 1/(2 b v)] \text{ERF}(b^{1/2} v) + 1/(b \pi)^{1/2} \text{Exp}(-b v^2)$$

Average Relative Speed

For verification we also need the average relative speed,

$$\langle v_r \rangle = \langle v_r K^*(v, v_r) \rangle / \langle K^*(v, v_r) \rangle$$

$$K^*(v, v_r) = (b/\pi)^{1/2} (v_r^2/v) \{ \text{Exp}[-b(v - v_r)^2] - \text{Exp}[-b(v + v_r)^2] \}$$

$$\langle v_r \rangle = \langle (b/\pi)^{1/2} (v_r^3/v) \{ \text{Exp}[-b(v - v_r)^2] - \text{Exp}[-b(v + v_r)^2] \} \rangle / \langle K^*(v, v_r) \rangle$$

Changing variables,

$$\begin{aligned} y^2 &= b v^2 \\ x^2 &= b v_r^2 \end{aligned}$$

$$\langle v_r \rangle = (1/b \pi)^{1/2} / y \langle x^3 \{ \text{Exp}[-(x - y)^2] - \text{Exp}[-(x + y)^2] \} d(x) \rangle / \langle K^*(v, v_r) \rangle$$

$$\langle b^{1/2} v_r \rangle = \langle x \rangle = (1/\pi)^{1/2} / y \langle \{ \text{Exp}[-(x - y)^2] - \text{Exp}[-(x + y)^2] \} d(x) \rangle / \langle K^*(v, v_r) \rangle$$

$$\langle x \rangle = \langle x^*(y) \rangle - \langle x^*(-y) \rangle$$

$$\langle x^*(y) \rangle = (1/\pi)^{1/2} / y \langle x^3 \text{Exp}[-(x - y)^2] d(x) \rangle / \langle K^*(v, v_r) \rangle$$

Changing variables,

$$\begin{aligned} Z &= x - y \\ x &= Z + y \\ d(x) &= d(Z) \end{aligned}$$

$$\langle x^*(y) \rangle = (1/\pi)^{1/2} / y \langle (Z + y)^3 \text{Exp}[-Z^2] d(Z) \rangle / \langle K^*(v, v_r) \rangle$$

From the above solution of the Doppler broadening equation,

$$y \text{sig}(y) = \langle K^*(v, v_r) \rangle = [y + 1/(2y)] \text{ERF}(y) + 1/(\pi)^{1/2} \text{Exp}(-y^2)$$

$$\langle x^*(y) \rangle = (1/\pi)^{1/2} / y \int_{-y \text{ to infinity}} (Z^3 + 3yZ^2 + 3y^2Z + y^3) \text{Exp}[-Z^2] d(Z)$$

$$\langle x^*(-y) \rangle = (1/\pi)^{1/2} / y \int_{+y \text{ to infinity}} (Z^3 - 3yZ^2 + 3y^2Z - y^3) \text{Exp}[-Z^2] d(Z)$$

Integrating and adding $\langle x^*(y) \rangle$ and $\langle x^*(-y) \rangle$,

$$\langle x \rangle = [3/2 + y^2] / [y + 1/(2y)] \text{ERF}(y) + 1/(\pi)^{1/2} \text{EXP}(-y^2)$$

$$\langle b^{1/2} v_r \rangle = [3/2 + b v^2] / [b^{1/2} v + 1/(2b^{1/2} v)] \text{ERF}(b^{1/2} v) + 1/(\pi)^{1/2} \text{EXP}(-b v^2)$$

$$\langle v_r \rangle = [3/2/b + v^2] / [v + 1/(2b v)] \text{ERF}(b^{1/2} v) + 1/(b \pi)^{1/2} \text{EXP}(-b v^2)$$

Low and High v Limits

$$\begin{aligned} y \operatorname{sig}(y) &= [y + 1/(2y)] \operatorname{ERF}(y) + 1/(\pi)^{1/2} \operatorname{Exp}(-y^2) \\ \langle x \rangle &= [3/2 + y^2]/[y + 1/(2y)] \operatorname{ERF}(y) + 1/(\pi)^{1/2} \operatorname{EXP}(-y^2) \\ b &= A/(2 k T) \end{aligned}$$

Low

$$\operatorname{ERF}(y) = 2/(\pi)^{1/2} \operatorname{Exp}(-y^2)[y + (2/3)y^3 + \dots]$$

$$\begin{aligned} \lim_{y \rightarrow 0} [y + 1/(2y)] \operatorname{ERF}(y) &\rightarrow 2/(\pi)^{1/2} \operatorname{Exp}(-y^2)[1/2 + (1/3)y^2 + y^2 + \dots] \\ &\rightarrow 1/(\pi)^{1/2} \operatorname{Exp}(-y^2) \end{aligned}$$

$$y \operatorname{sig}(y) \rightarrow 2/(\pi)^{1/2} \operatorname{Exp}(-y^2) \rightarrow 2/(\pi)^{1/2}$$

$$\begin{aligned} v \operatorname{sig}(v) &\rightarrow 2/(b \pi)^{1/2} \\ &\rightarrow [2/\pi^{1/2}] [2 k T/A]^{1/2} \end{aligned}$$

$$\langle x \rangle \rightarrow [3/2 + y^2]/[2/(\pi)^{1/2} \operatorname{Exp}(-y^2)] \rightarrow (3/2)[\pi^{1/2}/2]$$

$$\begin{aligned} \langle v_r \rangle &\rightarrow (3/2)/[(\pi/b)^{1/2}/2] \\ &\rightarrow (3/2)/[\pi^{1/2}/2][2 k T/A]^{1/2} \end{aligned}$$

In the low energy limit as the neutron Lab speed, v , approaches zero both the reaction rate, $v \operatorname{sig}(v)$, and the average relative speed, $\langle v_r \rangle$, approach constants. This is what we expect, since in this limit both are defined only by the thermal motion of the target. Note, that both have exactly the same $[T/A]^{1/2}$ dependence on temperature and target mass, i.e., they increase as temperature increases and decrease as target mass increases.

Note, since the low energy reaction, $v \operatorname{sig}(v)$, approaches a constant, the Doppler broadened cross section, $\operatorname{sig}(v)$, is varying as $1/v$.

High

$$\lim_{y \rightarrow \infty} \operatorname{ERF}(y) \rightarrow 1, \operatorname{Exp}(-y^2) \rightarrow 0$$

$$y \operatorname{sig}(y) \rightarrow [y + 1/(2y)] \rightarrow y$$

$$v \operatorname{sig}(v) \rightarrow v$$

$$\langle x \rangle \rightarrow [3/2 + y^2]/y \rightarrow y$$

$$\langle v_r \rangle \longrightarrow v$$

In the high energy limit as the neutron speed, v , becomes much larger than the target speed there is no longer a significant spread in the distribution of relative speeds, and the relative speed, v_r , approaches the neutron Lab speed, v . This is what we expect, since in this limit both are defined only by the neutron motion.

Note, since the high energy reaction, $v \sigma(v)$, approaches v , the Doppler broadened cross section, $\sigma(v)$, is varying as 1 , i.e., it approaches the constant Relative frame cross section.

Sampling

With all of the above as background, we now come to the point of this paper: how do we sample the distribution to define the speed and direction of neutrons after an elastic collision. The distribution of relative speeds is,

$$P = v_r P(v_t) / \langle v_r P(v_t) \rangle$$

Here we assume a constant relative cross section, $\sigma(v_r)$, and that $P(v_t)$ is an isotropic Maxwellian,

$$P(v_t) d(v_t) = P^*(v_t) d(v_t) d(\mu) d(\phi) / (4 \pi)$$

$$P^*(v_t) d(v_t) = (4/\pi)^{1/2} b^{3/2} v_t^2 \text{Exp}(-b v_t^2) d(v_t)$$

which leads to the reaction rate and average relative speed,

$$\langle v_r P(v_t) \rangle = [v + 1/(2b v)] \text{ERF}(b^{1/2} v) + 1/(b \pi)^{1/2} \text{Exp}(-b v^2)$$

$$\langle v_r \rangle = [3/2b + v^2] / [(v + 1/(2b v)) \text{ERF}(b^{1/2} v) + 1/(b \pi)^{1/2} \text{EXP}(-b v^2)]$$

where the relative speed, v_r , can be defined in terms of neutron, v , and target, v_t , speeds and the cosine, μ , between the directions of the neutron and target,

$$v_r^2 = [v^2 - 2 \mu v v_t + v_t^2]$$

In dimensionless form,

$$y^2 = b v^2$$

$$x^2 = b v_r^2$$

$$z^2 = b v_t^2$$

$$P = x P^*(z) / \langle x P^*(z) \rangle$$

$$P^*(z) d(z) = 4/\pi^{1/2} z^2 \text{Exp}(-z^2) d(z)$$

$$\langle x P(z) \rangle = [y + 1/(2y)] \text{ERF}(y) + 1/\pi^{1/2} \text{Exp}(-y^2)$$

$$x^2 = [y^2 - 2 \mu y z + z^2]$$

The Most Widely Used Method

In the general case with an energy dependent cross section there is an advantage to changing variables from μ to x , so that we can express the Doppler broadening equation in terms of x , relative speed, and therefore the energy dependent cross section $\text{Sig}(x)$, or $\text{Sig}(v_r)$, directly in terms of the variable x in the equation. Therefore we next change variables from μ to x , using,

$$2 x d(x) = -2 y z d(\mu)$$

$$x P(x) = x^2 4/\pi^{1/2} z^2 \text{Exp}(-z^2) d(x) d(z)/(2 y z)$$

$$= x^2 2/\pi^{1/2} z \text{Exp}(-z^2) d(x) d(z)/y$$

$$= 1/(\pi^{1/2} y) x^2 d(x) \text{Exp}(-z^2) d(z^2)$$

By integrating over z we obtain a singly dimensioned integral in x , the relative speed, so that we can define the cross section only in terms of the relative speed.

$$= 1/(\pi^{1/2} y) x^2 d(x) \{ \text{Exp}[-(x-y)^2] - \text{Exp}[-(x+y)^2] \}$$

This is the form that most approaches to thermal scattering use: sample the above distribution in x and y , and use,

$$x^2 = [y^2 - 2 \mu y z + z^2]$$

to define μ ,

$$\mu = [y^2 + z^2 - x^2]/[2 y z]$$

The THERMAL Method

Here I will use a much simpler approach. Since in this case the cross section is constant there really isn't any advantage to changing variables from μ to x . Therefore I will sample the distribution directly,

$$P = x P^*(z)/\langle x P^*(z) \rangle$$

$$P^*(z) d(z) = 4/\pi^{1/2} z^2 \text{Exp}(-z^2) d(z)$$

$$\langle x P(z) \rangle = [y + 1/(2y)] \text{ERF}(y) + 1/\pi^{1/2} \text{Exp}(-y^2)$$

$$x^2 = [y^2 - 2 \mu y z + z^2]$$

With this approach $P^*(z)$ is simply an isotropic Maxwellian. The most straightforward approach is to sample the isotropic Maxwellian, $P^*(z)$, and then accept or reject on the relative speed, x . However, this approach is very inefficient, particularly for low neutron speeds; in the low neutron speed limit the efficiency is only 28 %.

A better approach suggested by Gene Canfield (again, thank you Gene) is to multiply and divide by $[y + z]$, neutron plus target speed,

$$P = [x/(y + z)] [(y + z) P^*(z)] / \langle x P^*(z) \rangle$$

and to sample $(y + z) P^*(z)$, and accept or reject on $x/(y + z)$. The advantage of this approach is an increase in efficiency. For low neutron speeds, x , the relative speed, y , approaches the target speed, z , and in the low neutron speed limit efficiency approaches 100 %. Similarly for high neutron speeds, x , the relative speed, y , approaches the neutron speed and efficiency approaches 100 %. As we will see later, the minimum efficiency is at x slightly larger than 1, where the efficiency is roughly 69 %. Overall compared to sampling $P^*(z)$ directly this approach almost doubles the sampling speed.

We must sample,

$$\begin{aligned} P^+(z) d(z) &= (y + z) P^*(z) d(z) = (y + z) 4/\pi^{1/2} z^2 \text{Exp}(-z^2) d(z) \\ &= y P_1(z) d(z) + P_2(z) d(z) \end{aligned}$$

where,

$$P_1(z) d(z) = 4/\pi^{1/2} z^2 \text{Exp}(-z^2) d(z) = \text{Maxwellian}$$

$$P_2(z) d(z) = 4/\pi^{1/2} z^3 \text{Exp}(-z^2) d(z) = 2/\pi^{1/2} (z^2) \text{Exp}(-z^2) d(z^2)$$

The integral of P_1 , the Maxwellian, is unity, and the integral of P_2 is $2/\pi^{1/2}$, and the integral of P^+ is $y + 2/\pi^{1/2}$. Therefore with probability $y/[y + 2/\pi^{1/2}]$ we sample from P_1 , and with probability $2/\pi^{1/2}/[y + 2/\pi^{1/2}]$ we sample from P_2 .

The basic idea of this approach isn't new. In principle this is the same approach used by the MCNP program (ref. 3), as far as modifying the rejection to be based on $v_r/[v + v_t]$. However, MCNP samples from the distributions after the transforming from μ to v_r , resulting in more complicated functions of both v and v_r that must be sample. With the THERMAL approach of sampling the target speed and direction directly, both P_1 and P_2 are only a function of a single variable, target speed, z .

Since both P_1 and P_2 are only a function of one variable it is relatively simple to develop a method to directly sample them with essentially no rejection; rejection at the 10^{-7} level for P_1 and no rejection for P_2 .

It's worth mentioning that this approach is more than just a mathematical trick to improve sampling efficiency. We can physically interpret P_1 and P_2 as the limiting high and low speed distributions, respectively.

$$\text{Lim } y \rightarrow 0 \quad x P(z) \rightarrow z P(z) = P_2(z)$$

$$\text{Lim } y \rightarrow \text{infinity} \quad x P(z) \rightarrow y P(z) = P_1(z)$$

That is to say that as the neutron speed, y , approaches zero the relative speed, x , approaches the target speed, z , and we will always sample from $P_2(z)$. Similarly, as the neutron speed, y , becomes much larger than the target speed, z , the relative speed, x , approaches the neutron speed, and we will always sample from $P_1(z)$. Therefore physically this approach separates the original single distribution into two distributions that we can recognize as the low and high speed limiting contributions to the overall distribution.

The sampling method I use is,

- 1) select either P_1 or P_2 .
- 2) sample z , the scaled target speed, from either P_1 or P_2 .
- 3) sample μ , the direction of motion of the target, from an isotropic distribution
- 4) define the relative speed,

$$x^2 = [y^2 - 2 \mu y z + z^2]$$

The original version of THERMAL always accepted this relative speed. This corresponds to the case of a $1/v$, not constant, cross section, and was an **error**. Rather than sampling,

$$P = x P^*(z) / \langle x P^*(z) \rangle$$

this was equivalent to replacing $P^*(z)$ by $P^*(z)/x$ and sampling,

$$P = [x P^*(z)/x] / \langle [x P^*(z)/x] \rangle = P^*(z) / \langle P^*(z) \rangle = P^*(z)$$

only sampling a Maxwellian. This is equivalent to assuming a $1/v$, rather than the intended constant cross section, which was an error in the original version of THERMAL.

The current version of THERMAL correctly handles the constant cross case by accepting or rejecting on $x/[y + z]$, [on rejection start over at 2), above] and the result is an unbiased sample of,

$$P = x P^*(z) / \langle x P^*(z) \rangle$$

Compared to the original version of THERMAL, adding acceptance/rejection to the current version of THERMAL actually makes the algorithm faster. This is because the efficiency of acceptance is always very high, and the low speed, P₂, treatment is somewhat faster than the high speed, P₁, treatment. The original treatment was equivalent to always using the P₁, Maxwellian, treatment, so adding the P₁ treatment has resulted in an overall improvement in speed.

Kinematics

What makes THERMAL run so fast is its treatment of kinematics; the above selection of target speed and direction are a relatively small part of the overall method.

THERMAL uses direction cosines, relative to the (x, y, z) axii. The direction cosines of the neutron are called (alpha, beta, gamma) and the components of the neutron speed are (v_x, v_y, v_z),

v_x = alpha v, similarly for v_y and v_z.

The target and relative speed direction cosines and speeds are named (alphi, betat, gammat), (v_{xt}, v_{yt}, v_{zt}), and (alphar, betar, gammar), (v_{xr}, v_{yr}, v_{zr}) respectively.

The target speed, v_t, is randomly sampled from a Maxwellian, and its direction cosines (alphi, betat, gammat) are randomly selected from an isotropic distribution, which define the components of the target speed (v_{xt}, v_{yt}, v_{zt}). The components of the relative speed are then defined by adding the contributions of the neutron and target,

v_{xr} = v_x - v_{xt}, similarly for the y and z components.

The relative speed is then,

$$v_r = [v_{xr}^2 + v_{yr}^2 + v_{zr}^2]^{1/2}$$

Assuming that v_r has been accepted, in the Center of Mass system the speed of the neutron and target are,

$$v_{cm-n} = A v_r / [A + 1]$$

$$v_{cm-t} = v_r / [A + 1]$$

Since we assume that scattering is isotropic in the Center of Mass system the three new direction cosines of the neutron in the Center of Mass after the collision will be completely random and uncorrelated to its original direction cosines. Therefore we can randomly select three direction cosines (alphacm, betacm, gammacm) and components of the speed of the neutron in the Center of Mass system,

$v_{x-cm-n} = v_{cm-n} \alpha_{cm}$, similarly for the y and z components.

The components of the final neutron speed are then defined by adding together the contributions of Center of Mass motion, randomly scattered neutron in the Center of Mass, and target speed,

$v'_x = [v_x + A\{v_{x-cm-n} + v_{xt}\}]/[A + 1]$, similarly for the y and z components.

The final neutron speed is,

$$v' = [v'^2_x + v'^2_y + v'^2_z]^{1/2}$$

and its direction cosines are,

$$\alpha' = v'_x/v'$$

$$\beta' = v'_y/v'$$

$$\gamma' = v'_z/v'$$

which completely describes the scattered neutron and ends the sample.

What makes this method fast is the use of vectors to deal with each component of the speed separately and avoiding the tradition method of scattering through a cosine relative to the original neutron Center of Mass direction of motion, and then having to transform the original neutron Center of Mass direction cosines through the scattering cosine to define new neutron Center of Mass direction cosines. This has to be done when dealing with anisotropic scattering, where the initial and final direction cosines are correlated, but it does not have to be done when the scattering is isotropic.

As described above, this problem can be completely avoided by using the components of the speed and assuming isotropic scattering in the Center of Mass system: just randomize the Center of Mass motion of the neutron and vectorially add the results.

High Energy Treatment

At low energy THERMAL includes thermal motion and solves the kinematics equations as described above. At higher energy THERMAL assumes no thermal motion and solves the equivalent equations described above. The transition between low and high energy treatments has been defined in THERMAL to insure a smooth transition between the two treatments. The transition point is a variable in THERMAL, which in the distributed version of THERMAL is $(1000)^{1/2}$ times the average thermal speed of a neutron in the medium that it is interacting with, i.e., this means 1000 times the average thermal neutron energy. For example, for a medium at room temperature, 300 Kelvin, or about 1/40 eV, the thermal treatment extends up to 1000 times the average energy, or about 25 eV. By this point the average relative speed differs from the neutron speed by only less than 0.1 %.

The equations used at high energy are identical to those described above, with the additional assumptions: 1) the target speed is zero, 2) which implies the relative speed is equal to the neutron Lab speed. These two assumptions means that we do not have to sample and reject on relative speed. In which case we immediately know that the center of mass speed of the neutron is,

$$v_{cm-n} = A v / [A + 1]$$

Again, since the scattering is isotropic in the center of mass system, we randomize the center of mass motion, and vectorially add together the contributions of Center of Mass motion, and randomly scattered neutron in the Center of Mass,

$$v'_x = [v_x + A \{v_{x-cm-n}\}] / [A + 1], \text{ similarly for the y and z components.}$$

The final neutron speed is,

$$v' = [v'^2_x + v'^2_y + v'^2_z]^{1/2}$$

and its direction cosines are,

$$\alpha' = v'_x / v'$$

$$\beta' = v'_y / v'$$

$$\gamma' = v'_z / v'$$

which completely describes the scattered neutron and ends the sample.

Note, the similarity of this high energy treatment to the low energy treatment (the equations are exactly the same if we set $v_t = 0$, $v_r = v$), and its simplicity. It is this simplicity that makes this high energy treatment so efficient: on an IBM-PC Pentium Pro 200 it can sample about 31 million scatters a minute. Even if you are not using the low energy THERMAL treatment you should not overlook the advantage of using the high energy treatment, all the way up to the highest energy where elastic scattering is isotropic in the center of mass system.

Summary of Assumptions and Approximations

It is important for the user to understand all of the assumptions I have used, so that you can understand the range of validity of the method. The assumption are,

Sampling the Target Distribution

1) The distribution of target nuclei is an isotropic Maxwellian; the so called free atom approximation.

2) At low energy the elastic scattering is constant. Note, for the high energy treatment there is no restriction on the energy dependence of the elastic cross section.

3) At high energy thermal motion is ignored.

Kinematics of Collisions

4) Scattering is isotropic in the center of mass system.

5) Scattering is elastic.

Those are the only assumptions and approximations used in the method.

What's Next?

One of the advantages of the THERMAL method is the simplicity of sampling the target and relative speed and direction. Compare the most widely used method of sampling the distribution in two independent variables,

$$P(x, y) = 1/(\pi^{1/2}y) x^2 d(x) \{ \text{Exp}[-(x-y)^2] - \text{Exp}[-(x+y)^2] \}$$

to the THERMAL method of directly sampling the target speed and direction from the given distribution of targets,

$$P = x P^*(z) / \langle x P(z) \rangle$$

$$\begin{aligned} P^*(z) d(z) &= 4/\pi^{1/2} z^2 \text{Exp}(-z^2) d(z) \\ \langle x P(z) \rangle &= [y + 1/(2y)] \text{ERF}(y) + 1/\pi^{1/2} \text{Exp}(-y^2) \end{aligned}$$

and accepting or rejecting on relative speed $x/[y + 2/\pi^{1/2}]$,

$$x^2 = [y^2 - 2 \mu y z + z^2].$$

First of all, in order to derive the equation for the most widely used method,

$$P(x, y) = 1/(\pi^{1/2}y) x^2 d(x) \{ \text{Exp}[-(x-y)^2] - \text{Exp}[-(x+y)^2] \}$$

we have to assume that the distribution of target nuclei is an isotropic Maxwellian. In principle all the THERMAL method says is sample from the distribution of target nuclei, whatever it is, and reject on relative speed.

With the THERMAL method we are looking at and directly sampling the distribution of target nuclei, which is only a function of a single speed, or energy, dependent variable. Currently THERMAL assumes that the distribution of target nuclei is an isotropic Maxwellian. However, in principle we could use any distribution of target nuclei and sample it.

What's next is to consider thermal scattering law data and see if it is possible to represent this data in a simpler form, where we can directly sample the distribution of target nuclei.

References

- 1) "Exact Doppler Broadening of Tabulated Cross Sections", by D. E. Cullen and C. R. Weisbin, Nuclear Science and Engineering: 60, 199-229 (1976)
- 2) "The 1994 ENDF Pre-processing codes", by D. E. Cullen, IAEA-NDS-39 International Atomic Energy Agency (IAEA), Vienna, Austria, January 1994; this report includes the latest documentation for the SIGMA1 code.
- 3) "MCNP - A General Purpose Monte Carlo Code for Neutron and Photon Transport, Version 3A," by J. F. Briesmeister, editor, La-7396-m, Rev. 2, Los Alamos National Laboratory

Quality Assurance

This routine is distributed with a driver program TESTER that allows users to verify correct implementation of THERMAL and to test each step in the calculations. For those users who have the PLOTTAB code results can be immediately viewed (for a copy of PLOTTAB contact the author).

Here TESTER will be used to verify the results of each step of the calculations. The steps that are verified include,

- 1) Sampling a Maxwellian distribution
- 2) Sampling the distribution of relative speed
- 3) Calculation of average relative speed
- 4) Time dependent thermalization
- 5) Time independent thermalization

Dimensionless Variables

When dealing with neutron thermalization it seems as if the equations involve an awful lot of different variables: neutron Lab speed, target speed, relative speed, temperature, the atomic weight of the target, etc., etc., etc. If one were to try to verify the accuracy of any computer program by using all combinations of these variables it would be an impossible task.

In fact the equations really only involve a few independent variables. For the calculation of Doppler broadened cross sections and relative speed it is convenient to express everything in dimensionless form as multiplies of AE/KT , where A is the atomic weight, E is an energy, K is Boltzmann's constant, and T is temperature. In this dimensionless unit the results are only a function of a few variables and it is relatively simple to verify the accuracy of a computer code or routine (such as this one); this is the approach used in this report.

Per Unit Speed or Energy

Since THERMAL uses speed, rather than energy, all of the following results are per unit speed. For the convenience of those readers who are used to using energy here are the important relationships that you should understand,

The **slowing down spectrum** will be $1/v = c \, d(v)/v$, rather than $1/E$,

$$c_1 \, d(E)/E = c_1 \, m \, v \, d(v)/v^2 = c_2 \, d(v)/v$$

The thermal **neutron density** will be a Maxwellian,

$$c_1 \, E^{1/2} \, \text{Exp}[-b \, E^2] \, d(E) = c_1 \, (m/2)^{1/2} \, v \, \text{Exp}[-bm v^2/2] \, d(mv^2/2)$$

$$= c_2 v^2 \text{Exp}[-b' v^2] d(v)$$

The thermal **neutron flux** will be v times a Maxwellian,

$$\begin{aligned} c_1 v E^{1/2} \text{Exp}[-b E^2] d(E) &= c_1 (m/2)^{1/2} v^2 \text{Exp}[-bm v^2/2] d(mv^2/2) \\ c_3 E \text{Exp}[-b E^2] d(E) &= c_2 v^3 \text{Exp}[-b' v^2] d(v) \end{aligned}$$

Normalization of Results

For comparison purposes all of the following figures illustrate both the expected results and the sampled results. For the results sampling a Maxwellian and relative speed results are normalized absolutely per sample. In these cases the expected and sampled results should lie exactly on top of one another with no bias. For the time dependent and time independent results I don't have the foggiest idea what the normalization should be for the expected results; I would have to run an actual transport calculation to determine the normalization. In these cases the expected results are normalized to agree with the maximum in the sampled results. In this case we expect the correct expected shape, but a slight bias causing sampled results to always lie slightly below the expected results. The reader should be aware of this normalization and not be disturbed by any slight bias in the magnitude of the expected and sampled results.

Sampling a Maxwellian

In dimensionless form a Maxwellian is,

$$\frac{4}{(\pi)^{1/2}} X^2 \exp(-X^2) d(X)$$

$$X = (b)^{1/2} v_t$$

$$b = A/2KT$$

A = atomic weight of target nuclei

K = Boltzmann's constant

T = temperature

Note, the advantage of using dimensionless variables. Rather than having to verify that we can sample a Maxwellian and define target speed, v_t , for various combinations of atomic weight and temperature, we need only verify that we can sample the dimensionless variable X. If we can accurately do this we will have verified that we can do this for any combination of variables.

Figure 1 compares an exact Maxwellian to the results obtained randomly sampling using the THERMAL algorithm. When methodically sampled the THERMAL algorithm reproduces the integral of a Maxwellian to within 0.0001 % and the differential to within 0.01 % over the entire range of X. Even when randomly sampled this figure illustrates the excellent agreement. On the left hand side of this figure the agreement is so good that it is hard to tell that there are two separate curves. On the right hand side of the figure we can see that across the important center of the Maxwellian even random sampling produces agreement to within about 0.1 %.

Bottom line: the results verify that the THERMAL algorithm can accurately sample a Maxwellian.

Sampling Relative Speed

In dimensionless form the distribution of relative speeds is,

$$1/(\pi)^{1/2} * Y^2 * \{ \text{Exp}[-(Y-X)^2] - \text{Exp}[-(Y+X)^2] \} * d(Y)/X$$

$X = (b)^{1/2} * V_n$ - Neutron laboratory speed

$Y = (b)^{1/2} * V_r$ - Relative speed between neutron and target

$$b = A/2KT$$

Again note, with dimensionless variables, this distribution is only a function of X and Y. What we have to demonstrate is that for various fixed values of X (neutron Lab speed) we can accurately sample Y (relative speed).

It is important to note I am not directly sampling this distribution. THERMAL samples a Maxwellian to define target speed, V_t , and an isotropic angular distribution to define the target direction cosines, and accepts or rejects on relative speed. The relative speed is defined as,

$$V_r^2 = [V_t^2 + V_n^2 + 2 * \text{COS} V_t * V_t * V_n]$$

Therefore a critical step in quality assurance is to verify that the sampling method used by THERMAL actually reproduces the above distribution of relative speeds.

The next three figures compare the exact distributions to the results obtained randomly sampling a Maxwellian to define target speed and an isotropic distribution and rejection on relative speed.

Figure 2 includes results for small values of $X = 0.001, 0.01, 0.1$ and 1 ; neutrons that are extremely sub-thermal up to thermal energy. Again the agreement is so good that it is difficult to tell there are two curves on each plot, except at the low and high ends of the distribution where the probability is extremely low, so that not too many samples occur = poor statistics.

Figure 3 includes results for $X = 2, 3, 4$ and 5 . Compared to the previous low X results, in this X range the shape of the distribution is changing as the effect of the second exponential, $\text{Exp}[-(Y+X)^2]$, is becoming progressively smaller and eventually becomes insignificant.

Figure 4 includes results for $X = 6, 7, 8$ and 10 . Compared to the previous results by this X range the second exponential is completely insignificant and there is no longer any significant low energy "tail" to the distribution. Note the agreement over the entire range of relative speeds, except at the low and high ends of the distribution where the probability is extremely low, so that not too many samples occur = poor statistics.

Calculation of Average Relative Speed

On the basis of the preceding results where it was verified that THERMAL can accurately sample the distribution of relative speeds, one could assume that it can also calculate the average relative speed. However, because of the importance of this quantity this will not be assumed - it will be verified.

In dimensionless form in the case of an elastic scattering cross section that is constant in the relative system the average relative speed can be written in the form,

$$\langle Y \rangle = \text{Sigcm} * \langle Y * P(Y) * d(Y) \rangle / \langle P(Y) * d(Y) \rangle$$

$$P(Y) * d(Y) = 1/(\pi)^{1/2} * Y^2 * \{ \text{Exp}[-(Y-X)^2] - \text{Exp}[-(Y+X)^2] \} * d(Y) / X$$

$$X = (b)^{1/2} * V_n - \text{Neutron laboratory speed}$$

$$Y = (b)^{1/2} * V_r - \text{Relative speed between neutron and target}$$

$$b = A/2KT$$

The solution is,

$$\langle Y \rangle = [3/2 + X^2] / [(X + 1/(2X)) \text{ERF}(X) + 1/(\pi)^{1/2} \text{EXP}(-X^2)]$$

Table 1 presents results for a wide range of incident neutron speeds (X). In each case for a fixed incident neutron energy (X) results were randomly sampled. In this case I used A = 1 (hydrogen) at room temperature (293 K), for incident neutron speed between 1/1000 and 100 times thermal speed (thermal speed = 2200 meters/second = 2.2D-03 cm/shake).

All results are for various multiplies of $[AE/KT]^{1/2}$.

Results include

- 1) V - incident neutron speed
- 2) $\langle V_n^* \rangle$ - average neutron speed after collision.
- 3) $\langle V_r \rangle$ - average relative speed.
- 4) $\langle V_t \rangle$ - average target speed.
- 5) $\langle V_r \rangle / V_n$ - the ratio of average relative speed to incident neutron speed.
Both sampled and exact results are presented.
- 6) $\%(S-E)/E$ - the per-cent difference between the sampled and exact results.
- 7) $\%Accept$ - the efficiency of relative speed acceptance
- 8) Sec. - running time in seconds (per million samples)

In this case the differences $\%(S-E)/E$ indicate that THERMAL can reproduce the correct average relative speed over the entire range to within about 0.1 % or better. Note, the dividing line between the low high energy treatment and high energy treatment (near $X = 30$) - by this point the average relative speed is less than 0.1 % of the incident neutron speed, $\langle V_r \rangle / \langle V \rangle$.

In this case the % acceptance $[\%Accept]$ is essentially 100 % at low and high neutron speeds and it has a minimum of about 69 % slightly above $x = 1$. As far as the overall running time, compared to the original THERMAL method, including rejection has actually improved the running time, e.g., in the original THERMAL report similar results are presented which showed that at low neutron speed it took about 10 seconds to sample 1 million events; it now takes less than 7 seconds.

Low and High Speed Sampling Times

The above test involves a lot of overhead to tally results and as such is not a true test of the speed of the method. TESTER's low and high speed sampling test only involves repeated calling THERMAL with the minimum amount of overhead. Running this test demonstrates that on an IBM-PC Pentium Pro 200 THERMAL can sample about 9 million scatters at low energy with thermal scattering and about 31 million a minute at high energy without thermal scattering.

Bottom line: the results verify that the THERMAL algorithm can accurately reproduce the correct average relative speed.

Pure Scattering, Infinite Medium - Time Dependent Results

In a pure scattering (no absorption), infinite medium the equation to solve is,

$$d[v N(v)]/d[t] + \text{sig}(v) v N(v) = \text{Int} [\text{sig}(v' \rightarrow v) v' N(v') d(v')] + S(v, t)$$

$\text{Int}[v] \text{sig}(v' \rightarrow v) = \text{sig}(v)$, implying no absorption, conservation of neutrons

This equation does not have a finite, **time independent** solution. It's easy enough to understand why: if we have a time independent source $S(v)$, we can think of this as adding the same number of neutrons to the system per unit time, and since they cannot disappear from the system, over time the number of neutrons in the system will approach infinity. If you prefer to think in terms of a **time independent** Monte Carlo calculation, consider sampling one source neutron and tracking it until it disappears from the system. Since there is no way for the neutron to disappear from the system, tracking even one source neutron will take an infinite amount of time, and the resulting flux distribution from even this one sampled neutron will approach infinity, as it continues moving from one energy to another in a Maxwellian distribution and thereby continues to contribute to the flux.

In order to simulate this situation it is necessary to perform a **time dependent** calculation, starting from any fixed source distribution of neutrons at time zero, and allowing the distribution to evolve into a Maxwellian distribution in the number density of neutrons (not, flux or reaction rate - number density). The following results are based on a source that is instantaneous at time zero and monoenergetic,

$$S(v, t) = \Delta(v - v_0) \Delta(t)$$

In the following examples neutrons were started at 1 keV, 40,000 times room temperature energy, 200 times room temperature speed, and are tracked in time as they approach a Maxwellian in neutron density. Starting at this energy we will see results using both the high energy THERMAL treatment without thermal scattering and the low energy treatment with thermal scattering. In each time interval the neutron flux is scored and presented on the following figures. Note, these results are neutron flux, so we expect the result to be neutron speed times a Maxwellian.

Note, this is a secular equilibrium situation, where the neutrons continue to scatter from one speed to another, but on average the reaction rate at each speed (causing neutrons to leave speed v) is exactly balanced by the reaction rate at all other energies (causing neutrons to arrive at speed v).

Verification

Figure 5 illustrates results for slowing down in hydrogen. The time step has been defined to be constant, approximately equal to the average time between collisions for thermal neutrons. As such the early time results involving higher speed collisions (more collisions

per second) include results only after the neutrons have undergone a number of collisions, i.e., don't expect to see anything that looks like the singly collided flux at the end of first time step. This figure shows results after each of the first 40 time steps. From this figure we can easily see the relaxation of the neutron flux into v times a Maxwellian (a Maxwellian neutron density). After about 20 time steps the distribution has completely relaxed. The results after the remaining time steps indicate that it remains stationary in this distribution. Additional time step results have been generated to insure that the distribution does stay in this form, as it will forever. The last portion of this figure shows the results across the important center of the distribution.

The amount of "noise" in this last portion is because we are looking at the results at the end of 10 successive time steps overlayed on top of one another and since each time step has been defined to be the average time between collisions at thermal energy each neutron doesn't have much of a chance to contribute to the flux and the result is a great deal of variance in the distribution.

Again, note, the normalization of the expected results is based strictly on the maximum of the sampled results, and therefore is slightly biased to lie above all of the sampled results near the peak of the distribution. As such the slight difference in the ratio from unity in the second figure does not indicate a real bias or problem with the results. If you "eyeball" in a properly normalized expected result as about 1 % lower than indicated on the figure, you can see that the sampled results across the important peak of the distribution are everywhere within about 1 % of the expected results.

Time Dependent with Absorption

We can also solve the time dependent equation with absorption. In this case we do not expect the distribution to relax into a Maxwellian and stay there forever. With absorption we expect the magnitude of distribution to decrease with time. If the absorption cross section is $1/v$, it means the absorption reaction rate is the constant at all speeds, $v \sigma(v) = \text{constant}$, so that the rate of absorption will be the same at all energies. In this case as long as the absorption cross section is not too large compared to the scattering cross section, the distribution will relax into a Maxwellian and then decrease in magnitude with time. However it will not shift in energy away from a Maxwellian, since the absorption will be uniform at all energies, and as long as the scatter is sufficiently large compared to the absorption it will keep renewing the Maxwellian shape as it decreases in magnitude.

Figure 6 illustrates slowing down in hydrogen with $1/v$ absorption. From this figure we can see the magnitude of the distribution decreasing with each time step, but no apparent shift or major distortion of the distribution from a Maxwellian neutron density.

Atomic Weight Dependence

The results using targets other than hydrogen (as used above), are similar to those obtained with hydrogen. The only difference is the time scale as which everything happens. For higher atomic weight targets the neutrons will have more collisions in order

to slow down and relax into a Maxwellian, but eventually they will relax into exactly the same Maxwellian shape found for slowing down in hydrogen.

Figure 7 illustrates slowing down in U^{238} without absorption. Due to the high atomic weight it takes many more time steps to thermal, but eventually once again we see a final distribution corresponding to a Maxwellian neutron density.

Absorption, Infinite Medium - Time Independent Results

In the case where there is absorption the time independent equation is,

$$\text{sig}_t(v) v N(v) = \text{Int} [\text{sig}(v' \rightarrow v) v' N(v') d(v')] + S(v)$$

$$\text{sig}_t(v) = \text{sig}(v) + \text{sig}_a(v)$$

$$\text{Int}[v] \text{sig}(v' \rightarrow v) = \text{sig}(v')$$

$\text{sig}_t(v)$ = total cross section

$\text{sig}(v)$ = elastic scattering cross section

$\text{sig}_a(v)$ = absorption cross section

$S(v)$ = time independent source

I present here time independent results using a constant relative elastic scattering cross section and a $1/v$ absorption cross section, which is a good representation of the low energy absorption cross section in many materials. In later figures I will also use a single level Breit-Wigner resonance to illustrate the importance of resonance absorption. In general the cross section used will be,

$$\text{sig}(v) = \text{Elastic} + \text{Capture } (v_{rt}/v) + \text{Res width}^2 / [\text{width}^2 + (v^2 - v_r^2)^2]$$

Elastic = Doppler broadened elastic cross section (relative cross section = constant = 1)

Capture = Magnitude of $1/v$ cross section, normalized at v_{rt} , room temperature speed

Res = Maximum of resonance

width = Width of resonance

v_r = Speed (energy) of resonance peak

As long as there is some absorption cross section this problem will lead to a finite, time independent solution. Starting from a monoenergetic neutron source well above thermal energy (at 1 keV) what we see is a typical slowing down spectrum, going over into a Maxwellian like distribution at lower energies. I say "Maxwellian like", because for a small amount of absorption the result will be very close to a Maxwellian, but as absorption is increased the spectrum will harden and significantly differ from a Maxwellian.

The following figures illustrate the neutron flux [v time neutron number density] that results from these calculations. Note, the results are compared to v times a Maxwellian, to simulate neutron flux, not density.

Verification

In figure 8 we consider room temperature hydrogen. The first two figures illustrate results with only elastic scattering and $1/v$ capture, where the capture is normalized to be $1/1000$ -

th the elastic cross section at room thermal energy. Since the capture is quite small, in this case we expect the result to be very close to a Maxwellian neutron number density (v Maxwellian flux), which is exactly what we see. The first figure shows results over the entire range, and the second shows results over the important middle of the distribution.

Again, note, the normalization of the expected results is based strictly on the maximum of the sampled results, and therefore is slightly biased to lie above all of the sampled results near the peak of the distribution. As such the slight difference in the ratio from unity in the second figure does not indicate a real bias or problem with the results. If you "eyeball" in a properly normalized expected result as about 1 % lower than indicated on the figure, you can see that the sampled results across the important peak of the distribution are everywhere within about 1 % of the expected results.

Capture Dependence

Figure 9 shows results for a variety of values of the capture: compared to the elastic, 1/1000-th, 1/100-th, 1/10-th, and 1, at room temperature thermal energy. Note, over a wide range of capture the magnitude of the spectrum scales as $1/\text{capture}$, and stays close to the expected v Maxwellian, until the capture becomes large. Since a $1/v$ cross section means the reaction (capture) rate is the same at all energies, $v \sigma(v) = \text{constant}$, this is the expected result, where a small amount of $1/v$ absorption doesn't shift the spectrum; it merely absorbs equally from all parts of the spectrum, decreasing the overall magnitude of the neutron flux. For larger values of capture the spectrum will harden and significantly deviate from a Maxwellian, as we can see from this figure.

Temperature Dependence

Figure 10 illustrates the effect of temperature. In this figure I have decreased and increased the temperature by an order of magnitude from room temperature to present results at 30, 300, and 3000 Kelvin. Decreasing temperature moves the spectrum into a range of higher capture cross sections, due to the $1/v$ capture used here, and conversely increasing temperature moves the spectrum into a range of lower capture cross section. One might expect that in this case the resulting spectrum would increase with temperature as the spectrum is moved progressively further away from the $1/v$ capture cross section. NOT!!! Remember $1/v$ capture means a constant capture rate at all energies, $v \sigma(v) = \text{constant}$. Therefore changes in temperature have no overall effect on the magnitude of the spectrum, i.e., it is merely shifted in energy to correspond to the temperature, which is exactly what we see in this figure.

These results may disturb anyone who is used to nuclear reactors being inherently nuclear stable, in the sense that any increase in temperature will tend to decrease the neutron flux and return the reactor to a stable condition. Not to worry; they are nuclear stable, but not due to the typical low $1/v$ absorption cross sections in fissile materials. A more important effect, not included in the above results, are low energy absorption resonances.

In order to illustrate this effect figure 11 includes temperature dependent results including a low energy absorbing resonance at about 0.25 eV. This resonance is at an energy

roughly 10 times more than room thermal energy, which means only $\sqrt{10}$ in speed above room thermal. The following figure illustrates that when even one low energy resonance is included increasing temperature leads to a decrease the neutron flux, and therefore an inherently nuclear stable situation. Note, the depression in the neutron flux near 0.007 cm/shake due to the absorbing resonance.

Atomic Weight Dependence

Increasing target atomic weight will cause neutrons to have more collisions in slowing down toward a Maxwellian. With a $1/v$ capture cross section, or constant reaction rate, $v \sigma(v) = \text{constant}$, at each collision there is a chance that the neutron will be absorbed and not reach thermal energies. The more collisions a neutron has the more chance it will be absorbed, and since with increasing target weight it will have more collisions, we expect to see atomic weight depend results.

The last two figures of this section illustrate results for target atomic weights, $A = 1, 10, 40$ and 100 . In this first case there is $1/v$ absorption and in the second case $1/v$ and resonance absorption. In both cases at high energies we see the expected increase with atomic weight in the $1/v$ slowing down spectrum, i.e., since for higher atomic weight neutrons lose less energy per collision, they have more collisions per unit energy and contribute more to the flux per unit energy. With only $1/v$ absorption (figure 12) we see only a moderate atomic weight dependence. With $1/v$ and resonance absorption (figure 13) we see a much stronger atomic weight dependence. In this case by thermal energy we see a decrease in the neutron flux with increasing atomic weight because fewer neutrons have survived the slowing down process through the resonance and must undergo even more collisions in attempting to relax into a Maxwellian.

If you look closely you will see something that you have only read about in textbooks. This problem is a monoenergetic source in an infinite medium, which leads to Placzek oscillations in the slowing down spectrum. This effect can only be seen clearly in the $A = 10$ results; the scoring bins are too coarse to resolve this effect for the higher atomic weights. For the $A = 10$ results note the discontinuity in the slowing down density near 0.4 cm/shake (near the upper speed limit of the figure). This is the discontinuity predicted by Placzek due to single collided neutrons not being able to scatter to lower energies.

Collision by Collision Results

In the original THERMAL report results were presented illustrating that the old THERMAL method, without rejection on relative speed, leads to a Maxwellian distribution when neutrons are tracked collision by collision. That is to say, a number of neutrons were each tracked through exactly the same number of collisions and the distribution of neutrons after each collision were presented in the original THERMAL report. The results as presented are correct, but misleading. Again, as stated above, the original THERMAL method was **erroneously** in that it was equivalent to assuming a $1/v$, not a constant cross section, and it was this assumption that led to the Maxwellian, as explained below.

With the new THERMAL method when neutrons are tracked collision by collision the result is not a Maxwellian; the result is the reaction rate times a Maxwellian,

$$v \sigma(v) M(v) dv$$

Only in the case of a $1/v$ cross section ($v \sigma(v) = \text{constant}$) will the results be a Maxwellian - which is exactly what the original THERMAL method was **erroneously** assuming, leading to the results presented in the original THERMAL report.

The reason that collision by collision results do not lead to a Maxwellian when starting from a constant relative cross section is because this does not correspond to the real physical situation. In the real physical situation neutrons at different energies are interacting at different rates, and only by considering time (not collision by collision) can we simulate the real situation.

Note, in the case of a $1/v$ cross section, $v \sigma(v) = \text{constant}$, the neutrons are interacting at the same rate at all energies, and on average moving along at the same collision by collision rate. That's why the original THERMAL method collision by collision resulted in a Maxwellian.

Bottom line: **The original THERMAL method is incorrect and should not be used.** The Maxwellian results presented in the original THERMAL report are misleading in the sense that these results correspond to assuming a $1/v$, not the constant relative cross section that was intended - Sorry about that sports fans!!!

Comments from THERMAL

Documentation

This routine is designed to be self-documenting, in the sense that the latest documentation for the routine is included as comment lines at the beginning of the routine. Reports, such as this one, are periodically published. However, the user should be aware that the comment lines within the routine are continuously updated to reflect the most recent status of the routine and these comment lines must always be considered the most recent documentation. Therefore the user is advised to always read the comment lines within the routine.

The remainder of this report consists of a listing of the documentation that appears at the beginning of the THERMAL routine.

SUBROUTINE THERMAL(ATWT,TEMPE)

C
C

NEUTRON THERMAL SCATTERING ROUTINE

C VERSION 95.1 (FEBRUARY 1995)

C VERSION 95.2 (SEPTEMBER 1995) *COMPLETELY REPLACES ORIGINAL
C 95.1 VERSION - WHICH ERRONEOUSLY
C CALCULATED RESULTS FOR A $1/V$,
C RATHER THAN CONSTANT, ELASTIC
C SCATTERING CROSS SECTIONS.

C

C Written by
C Dermott E. Cullen
C University of California
C Lawrence Livermore National Laboratory
C L-59
C P.O. Box 808
C Livermore, CA 94550
C U.S.A.

C

C Tele: 415-423-7359
C E. Mail: cullen1@llnl.gov

C

PURPOSE

C

C Calculate elastic scattering that is isotropic in the center of
C mass system. At low energies thermal motion will be included.
C At high energies the target nuclei are assumed to be stationary.
C The point of transition between low and high energies has been
C defined to insure a smooth transition.

C

C It is assumed that at low energy the elastic cross section is
C constant. At high energy the cross section can be of any form.

C

C You can use this routine for all energies where the elastic
C scattering is isotropic in the center of mass system. In most
C materials this will be a fairly high energy.

C

RELATED ROUTINES

C

C This routine is designed to be used in conjunction with the
C SIGMA1 method of Doppler broadening cross sections. It is assumed
C that the laboratory system cross sections you use in your Monte
C Carlo calculations have been pre-calculated using the SIGMA1
C method. See, Ref. 1 & 2 for SIGMA1 documentation.

C

C The approach used here is consistent with that used in the SIGMA1
C method of Doppler broadening cross sections. If you have used the
C SIGMA1 method of Doppler broadening cross sections the reaction
C rates that you obtain using this routine will be completely
C consistent. If you have not Doppler broadened your cross sections
C the low energy reaction rate calculated by this routine will be
C higher than those predicted by your cross sections.

C

C **WARNING**

C

C You must call THERM0 once to initialize parameters before you
C call this routine the first time - you need only call THERM0 once.

C

C **DYNAMIC PARAMETERS**

C

C ATWT = Target atomic weight in neutron mass units
C TEMPE = Target temperature in MeV, e.g., 293 K = 2.53d-08 MeV
C (to use temperature in Kelvin see the below instructions)
C VNOW = Neutron speed in cm/shake (shake=1.0-8 seconds)
C (see THERM0 if you are using any other units)
C ALPNOW = Neutron direction cosine relative to X axis
C BETNOW = Neutron direction cosine relative to Y axis
C GAMNOW = Neutron direction cosine relative to Z axis

C

C **PARAMETER INTERFACE**

C

C This routine passes ATWT and TEMPE as arguments and the remaining
C variables are passed through COMMON/WHERENOW/. If you wish to use
C a different convention you need merely add additional variables
C as arguments and delete COMMON/WHERENOW.

C

C **STATIC PARAMETERS**

C

C EROOM = 2.53D-08 MeV (room temperature thermal energy)
C VROOM = 2.20D-03 cm/shake (room temperature thermal speed)
C VNMIN = 5.00D-04 cm/shake (minimum TART speed)
C (see THERM0 if you are using any other units)
C VNMAX = SQRT(1000.0) - at higher incident speeds ignore
C thermal motion - this means up to 1000 times the
C average thermal energy.

C

C **COMPLETE ISOTROPIC ELASTIC SCATTERING**

C

C This routine will handle elastic scattering at the energies where
C scattering is isotropic in the center of mass system. At lower
C incident energies thermal motion will be included. At higher
C incident energies thermal motion will not be included. The

dividing line between the two treatments is controlled by (VNMAX), presently defined to be $\text{SQRT}(1000)$. When the incident neutron speed is greater than (VNMAX) times the average thermalized neutron speed thermal motion is not included; otherwise it is included.

(VNMAX) has been defined to insure a smooth transition between the high and low energy treatments. For $(\text{VNMAX}) = \text{SQRT}(1000)$, the incident energy must be 1000 times the temperature of the medium, e.g., at room temperature of 0.0253 eV, thermal motion will be included up to about 25 eV. By this energy the average relative speed between neutron and target is within 0.1 % of the neutron speed.

ASSUMPTIONS AND RESTRICTIONS

It is assumed that at low energy in the relative frame the elastic scattering cross section is constant and that the target nuclei are distributed in an isotropic Maxwellian in the laboratory system, i.e., the so called free atom assumption.

For light isotopes the elastic cross section is constant to fairly high energy, so that this assumption is valid to describe the important slowing down in moderators. For heavy isotopes this assumption may no longer be valid above the eV energy range, but will be valid near thermal energies.

For a number of important moderators binding effects are very important, so that the free atom assumption is no longer valid. I recommend that you use the ENDF/B thermal scattering law data whenever possible. However, since thermal scattering law data is only available for a relatively small number of materials, in cases where this data is not available I recommend that you use this routine as an approximation to thermalization.

ISOTROPIC VS. NON-ISOTROPIC ELASTIC SCATTERING

Isotropic elastic scattering in the center of mass system allows the calculations to be greatly simplified and sped up. In this case the contributions of the neutron and target to the motion of the center of mass remain fixed through the collision (as they always do) and the motion of the neutron in the center of mass becomes random in direction.

In this case all we need do is randomize the center of mass direction of the neutron (randomly select 3 new direction cosines that are completely uncorrelated to the original direction cosines

C of the neutron) and then vectorially add it to the motion of
C the center of mass to define new laboratory neutron speed and
C directions; we do not have to worry about scattering through a
C given angular distribution, where the final direction cosines are
C correlated to the original direction cosines, and the subsequent
C transformation back to the laboratory system.

C This approach is valid at both high and low energies; the only
C difference between the two treatments being that at high energy
C the target is assumed to be stationary, so that its motion is not
C included in the vectorial addition used to define the new neutron
C speed and directions.

C **RUNNING TIME**

C On an Pentium Pro 200 the high energy treatment can sample over 31
C million histories in per minute and the low energy treatment can
C sample about 9 million histories per minute.

C **UNITS**

C As distributed this routine assumes energy in MeV and speed in
C cm/shake. Everything is normalized to the variables,
C EROOM = 2.53D-08 MeV (room temperature thermal energy)
C VROOM = 2.20D-03 cm/shake (room temperature thermal speed)
C VNMIN = 5.00D-04 cm/shake (minimum TART speed)

C To use any other units (e.g., eV and cm/second) all you need do is
C re-define these constants (see, ENTRY THERM0).

C **USING KELVIN TEMPERATURE**

C If you temperature is in Kelvin, instead of energy, activate
C the coding at the end of this routine to re-define BROOM.
C BROOM is used to normalize input temperature to room temperature.
C As presently defined it uses room temperature energy, EROOM,
C in MeV to do this, which is appropriate for input temperature in
C MeV. For input temperature in Kelvin all you have to do is use
C room temperature in Kelvin, TROOM, instead of room temperature
C energy, EROOM. See, the presently commented out coding at the
C end of this routine to do this.

C **MINIMUM ALLOWABLE SPEED**

C You do not want to accept speeds which are below the minimum
C energy of your neutron cross section data - any events that
C result in a lower speed will be rejected.

C
C See THERM0, which includes the minimum allowable speeds for users
C of the TART-175 group structure (minimum energy 1.307D-09 MeV),
C ENDL (minimum energy 1.0D-10 MeV) or ENDF/B (minimum energy
C 1.0D-11 MeV). If you are using one of these merely select the
C correct one in THERM0. If you are using some other data set you
C will have to either define the minimum in THERM0, or set the
C minimum in THERM0 to 0.0 and handle these cases as they are
C returned to you by this routine. If you do nothing you will be
C using the TART minimum allowable speed by default.

C C **PRECISION**

C
C This routine treats everything in REAL*8 = double precision on
C workstations, single precision on a CRAY. I recommend that you
C only use this routine in REAL*8 - otherwise CAVEAT EMPTOR!!!!

C C **RANDOM NUMBER GENERATOR**

C
C The distributed version of this routine uses a random number
C generator - RANF() - if this is not the random number generator
C used on your computer you need merely change RANF() to the name
C of your random number generator - remember, whatever routine you
C use must be REAL*8.

C C **SAMPLING A MAXWELLIAN**

C
C A good approximation to sampling a Maxwellian is to randomly
C select X using,

C
C $X = \text{Sqrt}(-\text{Log}(R1*(1-R2**2)))$, R1 and R2 random numbers

C
C The Maxwellian and the distribution resulting from the above
C distribution were equated,

C
C
$$F(Y)*d(Y) = G(X)*d(X)$$

C
C Integrating,

C
C
$$F(Y) = G(X)$$

C
C The sampled values of X from the above distribution were fit
C to reproduce the sampled values of Y from the Maxwellian,

C
C
$$Y = X/(((C3MAX*X+C2MAX)*X+C1MAX)*X+C0MAX)$$

C
C The result is a sampling method that reproduces the integral

C of a Maxwellian to better than 0.0001 % and the differential
C Maxwellian to better than 0.01 % over the entire range.

C
C The last step is to reject extremely low probability large
C values of Y. In the distributed version of this routine the
C rejection is controlled by XMAX which is = 4. The integral of
C a Maxwellian up to X = 4 is 1 - 5.0D-07, i.e., the probability
C of sampling an X above 4 is 5.0D-07, so that sampling efficiency
C is essentially 100 %.

C C **METHOD**

C
C The Doppler broadening equation is,

C
C
$$V * \text{Sig}(V) = \text{INT}[0, \text{INFINITY}] V_r * \text{Sig}(V_r) * P(V_r) * d(V_r)$$

C
C The distribution of relative speeds is defined by,

C
C
$$P(V_r) = V_r * \text{Sig}(V_r) * P(V_t) * d(V_t) / [V * \text{sig}(V)]$$

C
C This is the distribution that must be sampled. This distribution
C is closely related to the Doppler broadening equation. We will
C solve this equation by solving,

C
C
$$P = P(V_t) * d(V_t)$$

C
C and rejecting on $V_r * \text{Sig}(V_r)$, actually only on V_r , since we will
C assume that $\text{Sig}(V_r)$ is constant.

C
C The Doppler broadening equation is a conservation equation, where
C we want to define the Lab cross section, $\text{Sig}(V)$, to conserve the
C reaction rate that is occurring in the relative system; it is
C important to understand we are conserving reaction rate, not
C cross section.

C
C $P(V_r)$ must be defined such that,

C
C
$$V * \text{Sig}(V) = \langle V_r * \text{Sig}(V_r) \rangle = \langle V_r * \text{Sig}(V_r) * P(V_r) \rangle / \langle P(V_r) \rangle$$

C
C produces the correct average reaction rate $\langle V_r * \text{Sig}(V_r) \rangle$, in
C which case we will have properly defined the Lab, Doppler
C broadened cross section, $\text{Sig}(V)$, to obtain the same observed
C reaction rate in Lab and relative systems.

C
C The starting point for deriving the above equation is,

C
C
$$V * \text{Sig}(V) = \text{INT}[-1, +1] d(\text{COS}) / 2 * \text{INT}[V_t: V_r > 0] V_r * \text{Sig}(V_r) * P(V_t) d(V_t)$$

C where the 2 integrals are over the target angular and energy
 C distributions. The only assumption is that the target distribution
 C is isotropic. We can rewrite this in the form,
 C
 C $V * \text{Sig}(V) = \text{INT}[\text{COS}] \text{INT}[V_t] V_r * \text{Sig}(V_r) d(\text{COS}) / 2 * P(V_t) d(V_t)$
 C
 C In which case the proper $P(V_r) d(V_r)$ to use is,
 C
 C $d(\text{COS}) / 2 * P(V_t) d(V_t)$
 C
 C In the general case with an energy dependent cross section $\text{Sig}(V_r)$
 C sampling this distribution will sample $V_r * \text{Sig}(V_r)$ and it is very
 C difficult to separate the two and define V_r and $\text{Sig}(V_r)$. However,
 C in the case of a constant cross section this distribution will
 C sample V_r ; based on the sampled target speed V_t and direction
 C COS we can immediately define the relative speed V_r and direction,
 C
 C $V_r = \text{Sqrt}[V_t^2 + V^2 + 2 * \text{COS} * V * V_t]$
 C
 C with no preferential treatment of any V_r . In this case there are
 C no restrictions on the range of COS and V_t , i.e., we can sample
 C any V_t and still be able to sample the entire range of COS such
 C that we can always define a relative speed.
 C
 C In other words independently sample the isotropic angular
 C distribution $d(\text{COS}) / 2$ and the distribution of target speeds
 C $P(V_t) d(V_t)$ to define a relative speed, V_r . I say "a" rather than
 C "the" relative speed because we will accept/reject V_r , as
 C described below.
 C
 C Note, this is a general result which applies to any isotropic
 C target distribution (isotropic, so that the angular and
 C energy distributions are not correlated). Here I will assume
 C $P(V_t) d(V_t)$ is a Maxwellian, in which case we have the familiar
 C Doppler broadening equation,
 C
 C $V * \text{Sig}(V) = \text{INT}[0, \text{INFINITY}] V_r * P(V_r) * d(V_r)$
 C
 C $P(V_r) * d(V_r) = C * (V_r / V) * [\text{Exp}(-(V - V_r)^2) - \text{Exp}(-(V + V_r)^2)]$
 C
 C $V * \text{Sig}(V) = \langle V_r * P(V_r) * d(V_r) \rangle / \langle P(V_r) * d(V_r) \rangle$
 C $\quad \quad \quad = \langle V_r \rangle$
 C
 C $\text{Sig}(V) = \langle V_r \rangle / V$
 C
 C At high energies (speeds) where the target speed becomes

insignificant the relative speed approaches the neutron speed and the Doppler broadened cross section approaches a constant. At low energies (speeds) where the neutron speed becomes insignificant the relative speed approaches the average target speed (a constant) and the Doppler broadened will increase; at very low energies it will increase as $1/V$.

LOW SPEED

The target nuclei are distributed as a Maxwellian,

$$\begin{aligned} \text{Maxwellian} &= 4/\text{Sqrt}(\text{Pi}) * B^{3/2} * V_t^{*2} * \text{Exp}(-B * V_t^{*2}) * d(V_t) \\ B &= ATWT/(2 * KT) \\ X &= \text{Sqrt}(B) * V_t \\ d(X) &= \text{Sqrt}(B) * d(V_t) \\ \text{Maxwellian} &= 4/\text{Sqrt}(\text{Pi}) * X^{*2} * \text{Exp}(-X^{*2}) * d(X) \end{aligned}$$

We must sample,

$$P = V_r * \text{Maxwellian}$$

To improve sampling efficiency multiply and divide by $[V + V_t]$. The result is two distributions,

$$P = [V_r / (V + V_t)] [V * P_1 + P_2]$$

$$P_1 = \text{Maxwellian}$$

$$P_2 = V_t * \text{Maxwellian}$$

We will sample $[V * P_1 + P_2]$ and reject on $[V_r / (V + V_t)]$.

The integral of P_1 is unity and the integral of P_2 is $2/(B * \text{PI})^{*1/2}$ and the integral of $[V * P_1 + P_2]$ is $V + 2/(B * \text{PI})^{*1/2}$.

Therefore with probability $V/[V + 2/(B * \text{PI})^{*1/2}]$ we will sample from P_1 , otherwise we will sample from P_2 .

The entire sampling procedure is then,

- 1) Select either P_1 or P_2 to sample.
- 2) Sample the target speed V_t from P_1 and P_2 .
- 3) The target nuclei are isotropic in the lab system. Sample to define the target direction cosines (AT, BT, GT)

C 4) The relative speed is,

C

$$C \quad VRX = ALPNOW * VNOW - AT * VT$$

$$C \quad VRY = BETNOW * VNOW - BT * VT$$

$$C \quad VRZ = GAMNOW * VNOW - GT * VT$$

$$C \quad VR^{**2} = VRX^{**2} + VRY^{**2} + VRZ^{**2}$$

C

C 5) Accept or Reject on relative speed. If rejected start over
C at 2), otherwise proceed to 6).

C

C 6) Isotropically scatter in the center of mass system. Randomly
C sample relative direction cosines (AS, BS, GS).

C

C In the center of mass system,

$$C \quad VNCM = VR * ATWT / (1 + ATWT) = \text{Center of mass neutron speed}$$

$$C \quad VCM = VR / (1 + ATWT) = VR - VNCM = \text{Center of mass speed}$$

C

C Note, in the following equations the factor $1/(1+ATWT)$ is
C omitted, except in the definition of the final neutron speed.

C

C 7) Vectorially add the center of mass, neutron and target speeds to
C define new components of the neutron speed,

C

$$C \quad VX' = [ALPNOW * VNOW + ATWT * (AS * VR + AT * VT)]$$

$$C \quad VY' = [BETNOW * VNOW + ATWT * (BS * VR + BT * VT)]$$

$$C \quad VZ' = [GAMNOW * VNOW + ATWT * (GS * VR + GT * VT)]$$

C

C 8) The new neutron speed is,

C

$$C \quad VNOW' = \text{Sqrt}[VX'^{**2} + VY'^{**2} + VZ'^{**2}] / (1 + ATWT)$$

C

C and the new direction cosines are,

C

$$C \quad ALPNOW' = VX' / \text{SQRT}(VX'^{**2} + VY'^{**2} + VZ'^{**2})$$

$$C \quad BETNOW' = VY' / \text{SQRT}(VX'^{**2} + VY'^{**2} + VZ'^{**2})$$

$$C \quad GAMNOW' = VZ' / \text{SQRT}(VX'^{**2} + VY'^{**2} + VZ'^{**2})$$

C

C 9) If $VNOW'$ is less than the minimum acceptable speed ($VNMIN$),
C reject and start over at 1)

C

C Otherwise return the sampled values.

C

C HIGH SPEED

C

C The target nuclei are assumed to be stationary. The treatment
C is a simplified version of the low speed treatment with,

C

```

C   Vt = 0
C   Vr = Vn
C
C   1) Isotropically scatter in the center of mass system. Randomly
C       sample relative direction cosines (AS, BS, GS).
C
C   2) Vectorially add the center of mass and neutron speeds to define
C       new components of the neutron speed,
C
C       VX'  = [ALPNOW + ATWT*AS]
C       VY'  = [BETNOW + ATWT*BS]
C       VZ'  = [GAMNOW + ATWT*GS]
C
C   3) The new neutron speed is,
C
C       VNOW' = VNOW*SQRT[VX'**2 + VY'**2 + VZ'**2]/(1 + ATWT)
C
C       and the new direction cosines are,
C
C       ALPNOW' = VX'/SQRT(VX'**2 + VY'**2 + VZ'**2)
C       BETNOW' = VY'/SQRT(VX'**2 + VY'**2 + VZ'**2)
C       GAMNOW' = VZ'/SQRT(VX'**2 + VY'**2 + VZ'**2)
C
C   4) If VNOW' is less than the minimum acceptable speed (VNMIN),
C       reject and start over at 1)
C
C       Otherwise return the sampled values.
C
C   FINAL TARGET SPEED AND DIRECTION
C
C   If you are interested in the final target speed and direction,
C   e.g., neutrons incident on hydrogen producing protons, the
C   equations are very similar. In the center of mass system if
C   after the collision the neutron is moving with direction cosines
C   (+AS, +BS, +GS), the target is moving with direction cosines
C   (-AS, -BS, -GS).
C
C   Relative to the target the direction of the center of mass is
C   the reverse of that relative to the neutron.
C
C   All you need do is vectorially add the center of mass, neutron
C   and target speeds to define the final target speed (VXT',
C   VYT', VZT'), just as was done for the neutron to define (VX',
C   VY', VZ') and then the above equations can be used to define
C   the final target speed and directions.
C
C   Starting from the above equations, exchange neutron and target,

```


C and reverse the center of mass directions,

C

C $VXT' = [AT*VT - ATWT*(AS*VR + ALPNOW*VNOW)]$

C $VYT' = [BT*VT - ATWT*(BS*VR + BETNOW*VNOW)]$

C $VZT' = [GT*VT - ATWT*(GS*VR + GAMNOW*VNOW)]$

C

C That's the good news - the bad news is since this routine is

C restricted to isotropic scattering in the center of mass the

C energies involved will be relatively small and you will never

C have very energetic final targets - so this routine will be

C of little practical use to generate energetic targets, e.g.,

C for neutrons on hydrogen at these low energies you will never

C generate very energetic protons.

C

C REFERENCES

C

C 1) "Exact Doppler Broadening of Tabulated Cross Sections", by D. E. Cullen and

C C. R. Weisbin, Nuclear Science and Engineering: 60, 199-229 (1976)

C

C 2) "The 1994 ENDF Pre-processing codes", by D. E. Cullen, IAEA-NDS-39

C International Atomic Energy Agency (IAEA), Vienna, Austria, January 1994; this

C report includes the latest documentation for the SIGMA1 code.

C

All speeds are multiplies of [A/KT]**1/2

V	<Vn*>	<Vr>	<Vt>	<Vr>/<Vn> Sampled	<Vr>/<Vn> Exact	% (S-E)/E	% Accept	Sec.
1.000D-03	8.862D-01	1.329D+00	1.329D+00	1.329D+03	1.329D+03	-0.01	99.90	5.9
1.259D-03	8.876D-01	1.331D+00	1.331D+00	1.057D+03	1.056D+03	0.09	99.89	5.9
1.585D-03	8.854D-01	1.329D+00	1.329D+00	8.384D+02	8.388D+02	-0.04	99.86	5.8
1.995D-03	8.863D-01	1.329D+00	1.329D+00	6.662D+02	6.662D+02	0.00	99.82	5.5
2.512D-03	8.869D-01	1.330D+00	1.330D+00	5.294D+02	5.292D+02	0.04	99.78	5.6
3.162D-03	8.867D-01	1.329D+00	1.329D+00	4.204D+02	4.204D+02	0.01	99.73	5.9
3.981D-03	8.856D-01	1.329D+00	1.329D+00	3.337D+02	3.339D+02	-0.05	99.65	5.9
5.012D-03	8.864D-01	1.330D+00	1.330D+00	2.653D+02	2.652D+02	0.03	99.56	6.0
6.310D-03	8.859D-01	1.329D+00	1.329D+00	2.107D+02	2.107D+02	-0.01	99.44	6.0
7.943D-03	8.863D-01	1.329D+00	1.329D+00	1.673D+02	1.674D+02	-0.02	99.30	6.0
1.000D-02	8.857D-01	1.329D+00	1.329D+00	1.329D+02	1.329D+02	-0.01	99.12	5.7
1.259D-02	8.866D-01	1.330D+00	1.329D+00	1.056D+02	1.056D+02	0.01	98.91	5.4
1.585D-02	8.860D-01	1.329D+00	1.329D+00	8.388D+01	8.388D+01	0.00	98.64	5.9
1.995D-02	8.861D-01	1.329D+00	1.329D+00	6.663D+01	6.663D+01	-0.01	98.27	6.0
2.512D-02	8.863D-01	1.330D+00	1.329D+00	5.294D+01	5.293D+01	0.01	97.85	6.0
3.162D-02	8.863D-01	1.329D+00	1.329D+00	4.203D+01	4.205D+01	-0.05	97.32	6.0
3.981D-02	8.865D-01	1.330D+00	1.329D+00	3.340D+01	3.341D+01	-0.02	96.68	6.0
5.012D-02	8.872D-01	1.330D+00	1.329D+00	2.654D+01	2.655D+01	0.00	95.85	6.0
6.310D-02	8.874D-01	1.331D+00	1.329D+00	2.110D+01	2.110D+01	0.02	94.86	5.8
7.943D-02	8.881D-01	1.332D+00	1.328D+00	1.677D+01	1.677D+01	-0.01	93.57	5.7
1.000D-01	8.887D-01	1.333D+00	1.328D+00	1.333D+01	1.334D+01	-0.03	92.19	6.3
1.259D-01	8.902D-01	1.335D+00	1.326D+00	1.061D+01	1.061D+01	-0.07	90.39	6.2
1.585D-01	8.917D-01	1.339D+00	1.324D+00	8.448D+00	8.457D+00	-0.12	88.36	6.3
1.995D-01	8.966D-01	1.346D+00	1.323D+00	6.748D+00	6.750D+00	-0.02	86.12	6.4
2.512D-01	9.016D-01	1.355D+00	1.319D+00	5.396D+00	5.402D+00	-0.10	83.49	6.5
3.162D-01	9.115D-01	1.372D+00	1.314D+00	4.338D+00	4.341D+00	-0.07	80.71	6.7
3.981D-01	9.255D-01	1.396D+00	1.307D+00	3.507D+00	3.509D+00	-0.07	77.73	6.6
5.012D-01	9.458D-01	1.433D+00	1.296D+00	2.860D+00	2.863D+00	-0.09	74.87	6.5
6.310D-01	9.795D-01	1.491D+00	1.282D+00	2.363D+00	2.364D+00	-0.05	72.36	6.9
7.943D-01	1.029D+00	1.574D+00	1.261D+00	1.981D+00	1.984D+00	-0.14	70.31	7.3
1.000D+00	1.104D+00	1.699D+00	1.239D+00	1.699D+00	1.699D+00	0.01	69.11	7.4
1.259D+00	1.215D+00	1.874D+00	1.215D+00	1.488D+00	1.487D+00	0.07	69.01	7.5
1.585D+00	1.372D+00	2.113D+00	1.191D+00	1.333D+00	1.333D+00	0.01	69.95	7.3
1.995D+00	1.593D+00	2.442D+00	1.171D+00	1.224D+00	1.223D+00	0.06	71.85	6.9
2.512D+00	1.893D+00	2.882D+00	1.158D+00	1.147D+00	1.147D+00	0.05	74.40	6.4
3.162D+00	2.288D+00	3.465D+00	1.148D+00	1.096D+00	1.095D+00	0.06	77.44	7.1
3.981D+00	2.801D+00	4.226D+00	1.141D+00	1.062D+00	1.061D+00	0.04	80.35	7.0
5.012D+00	3.461D+00	5.208D+00	1.137D+00	1.039D+00	1.039D+00	0.01	83.30	6.8
6.310D+00	4.301D+00	6.466D+00	1.134D+00	1.025D+00	1.025D+00	0.01	85.93	6.7
7.943D+00	5.374D+00	8.068D+00	1.132D+00	1.016D+00	1.016D+00	0.00	88.26	6.5
1.000D+01	6.727D+00	1.010D+01	1.132D+00	1.010D+00	1.010D+00	0.00	90.31	6.1
1.259D+01	8.440D+00	1.267D+01	1.129D+00	1.006D+00	1.006D+00	0.00	92.07	6.0
1.585D+01	1.061D+01	1.591D+01	1.129D+00	1.004D+00	1.004D+00	-0.01	93.50	6.4
1.995D+01	1.333D+01	2.000D+01	1.129D+00	1.003D+00	1.003D+00	0.00	94.79	6.3
2.512D+01	1.678D+01	2.516D+01	1.128D+00	1.002D+00	1.002D+00	-0.01	95.77	6.4
3.162D+01	2.109D+01	3.162D+01	1.129D+00	1.000D+00	1.001D+00	-0.10	100.00	2.2
3.981D+01	2.654D+01	3.981D+01	1.129D+00	1.000D+00	1.001D+00	-0.06	100.00	2.1
5.012D+01	3.343D+01	5.012D+01	1.129D+00	1.000D+00	1.000D+00	-0.04	100.00	2.2
6.310D+01	4.206D+01	6.310D+01	1.129D+00	1.000D+00	1.000D+00	-0.03	100.00	2.1
7.943D+01	5.294D+01	7.943D+01	1.129D+00	1.000D+00	1.000D+00	-0.02	100.00	2.0
1.000D+02	6.668D+01	1.000D+02	1.129D+00	1.000D+00	1.000D+00	-0.01	100.00	2.0

Table 1: Calculation of relative speed versus fixed neutron speed

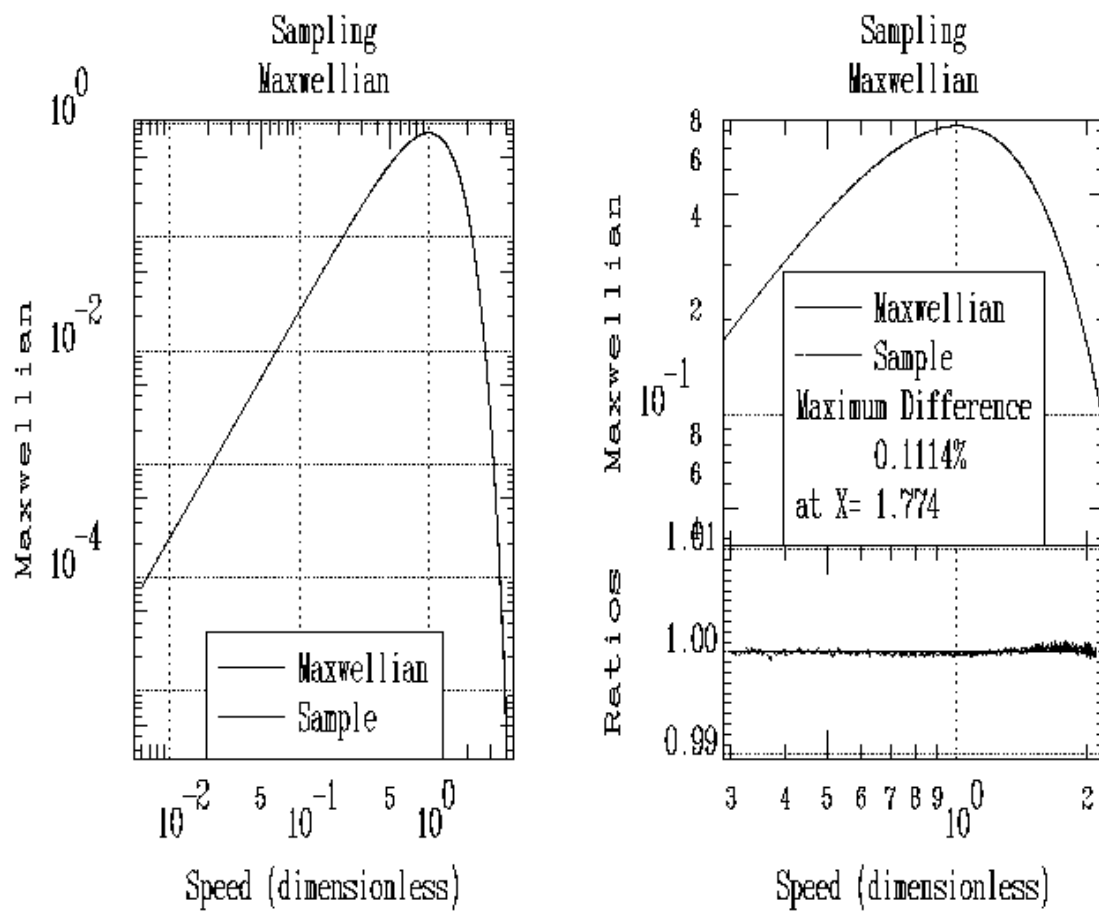


Figure 1: Sampling a Maxwellian

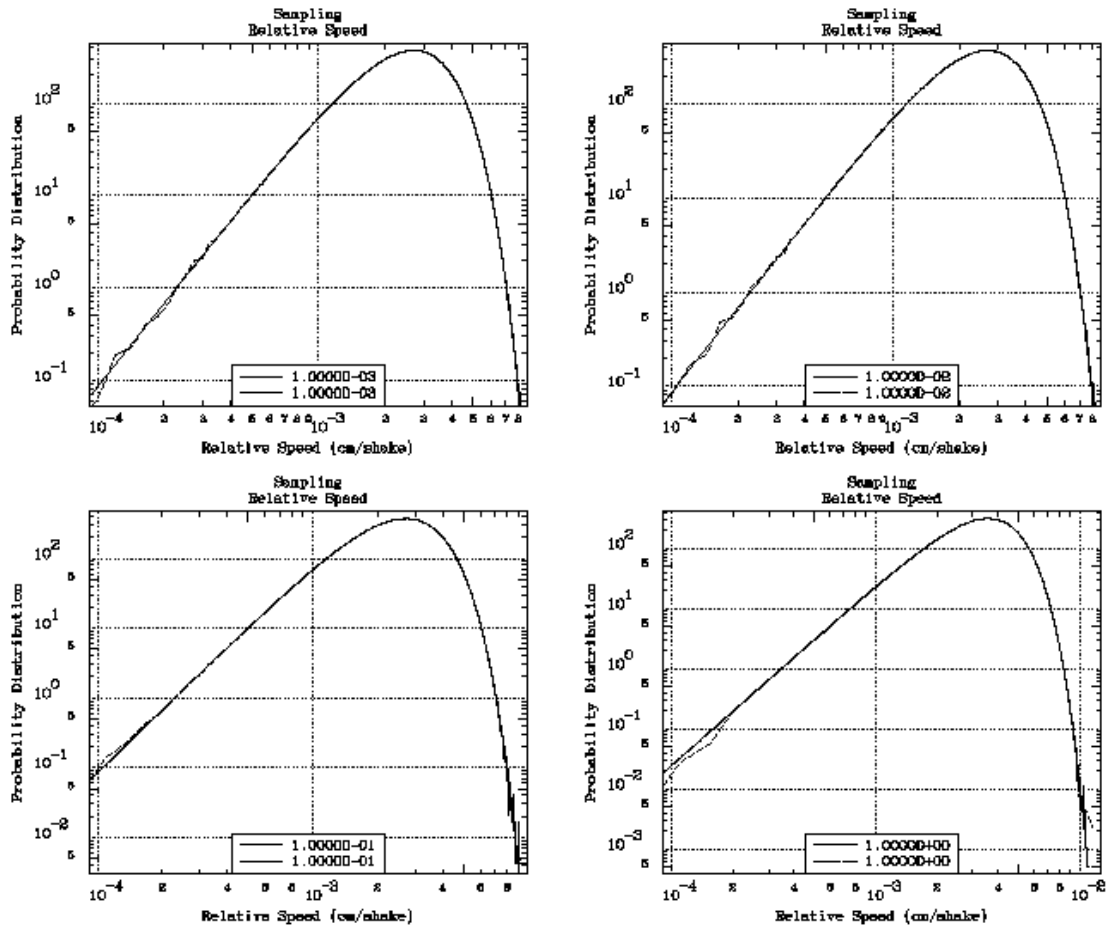


Figure 2: Sampling relative speed, $x = 0.001, 0.01, 0.1$, and 1

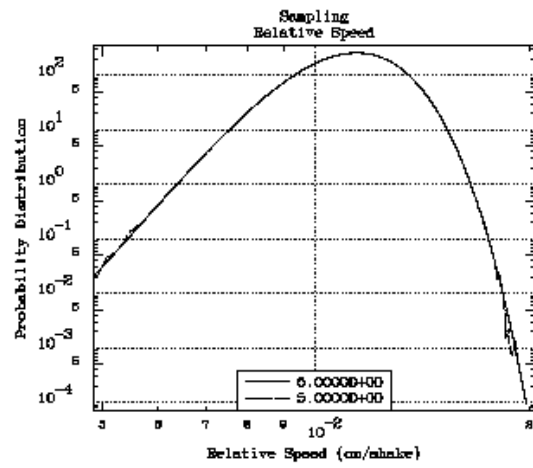
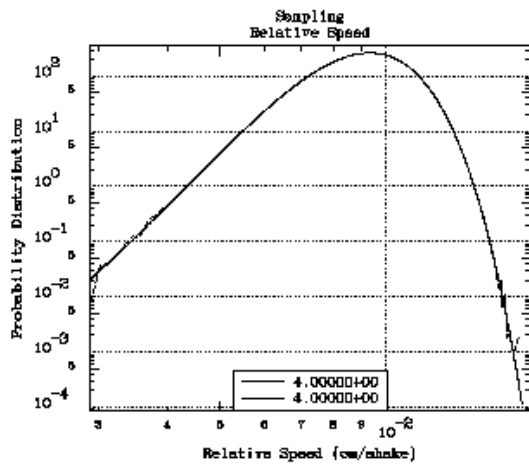
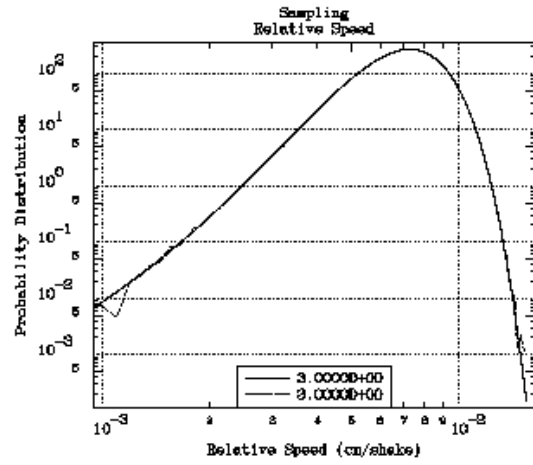
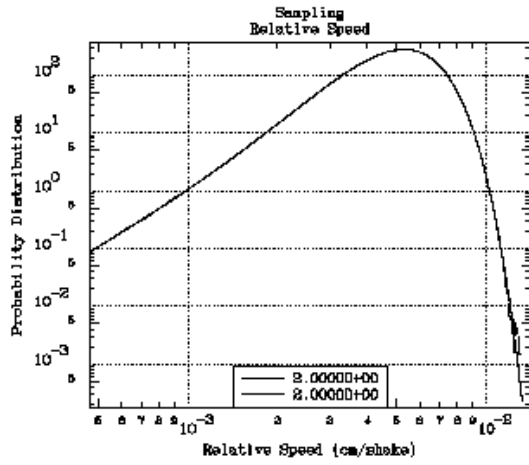


Figure 3: Sampling Relative Speed, $x = 2, 3, 4$, and 5

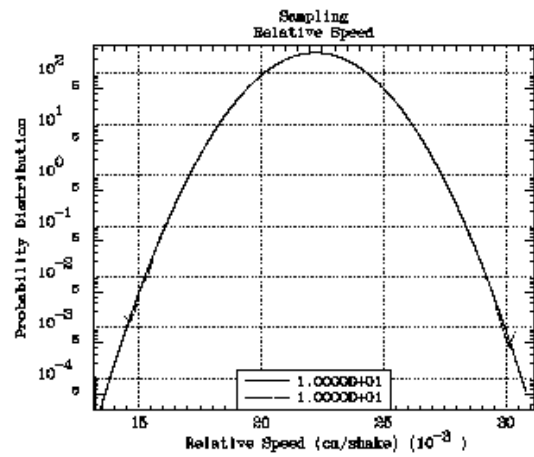
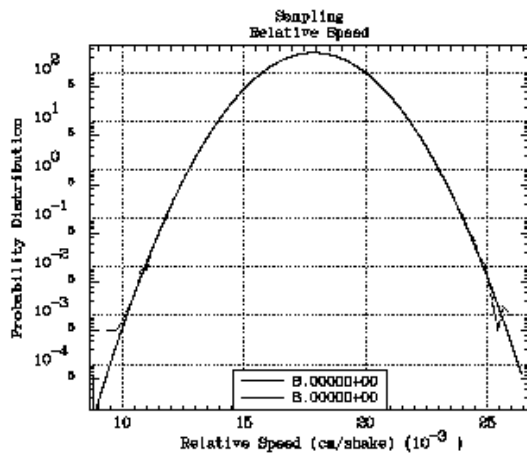
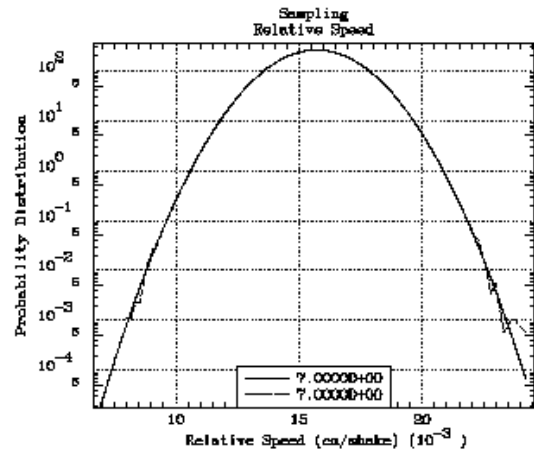
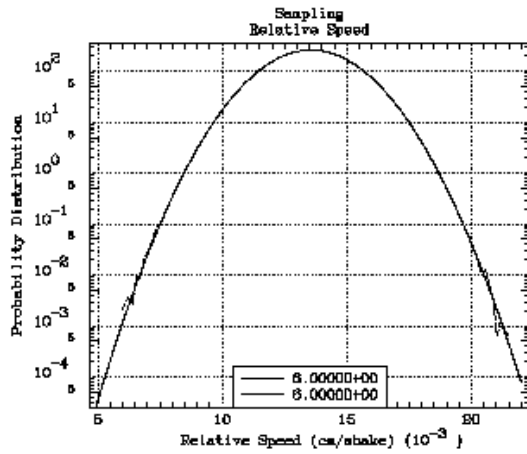


Figure 4: Sampling Relative Speed, $x = 6, 7, 8$, and 10

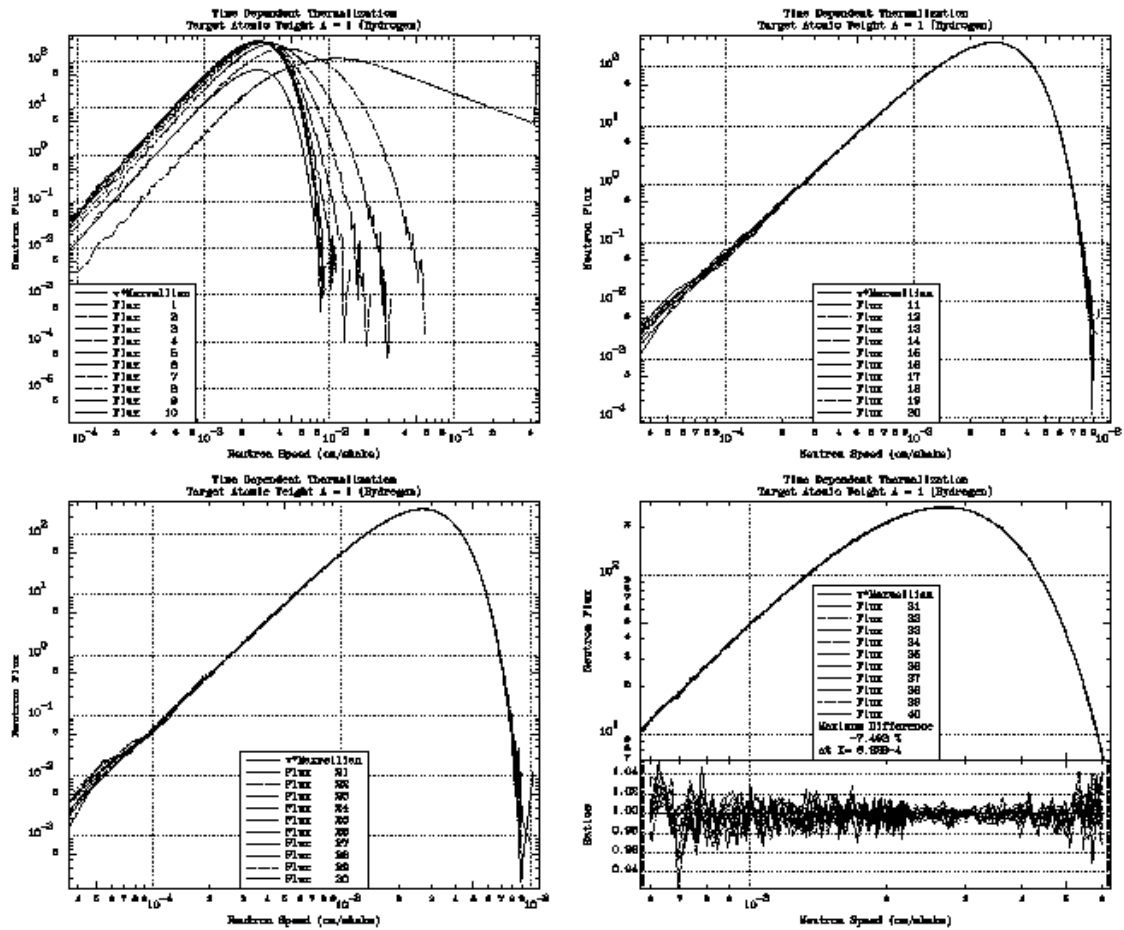


Figure 5: Time dependent thermalization without absorption; atomic weight = 1

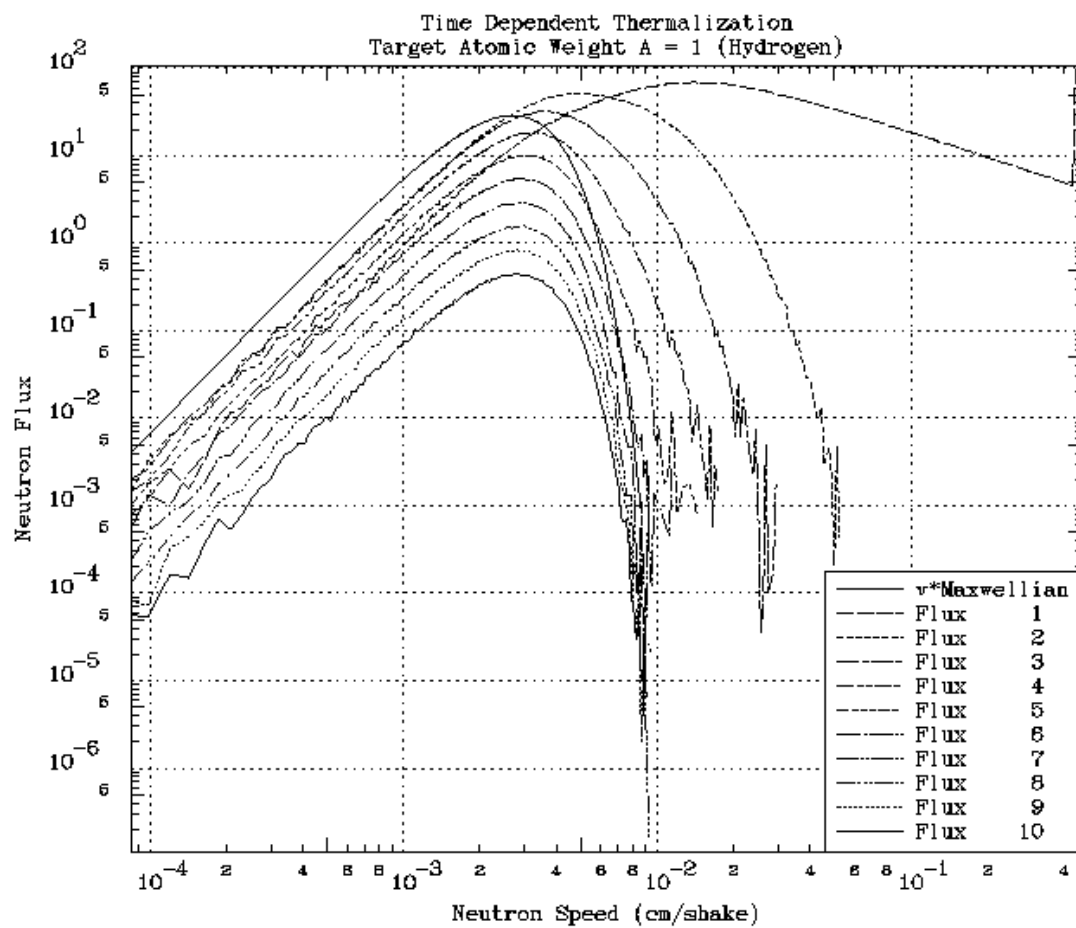


Figure 6: Time dependent thermalization with absorption; atomic weight = 1

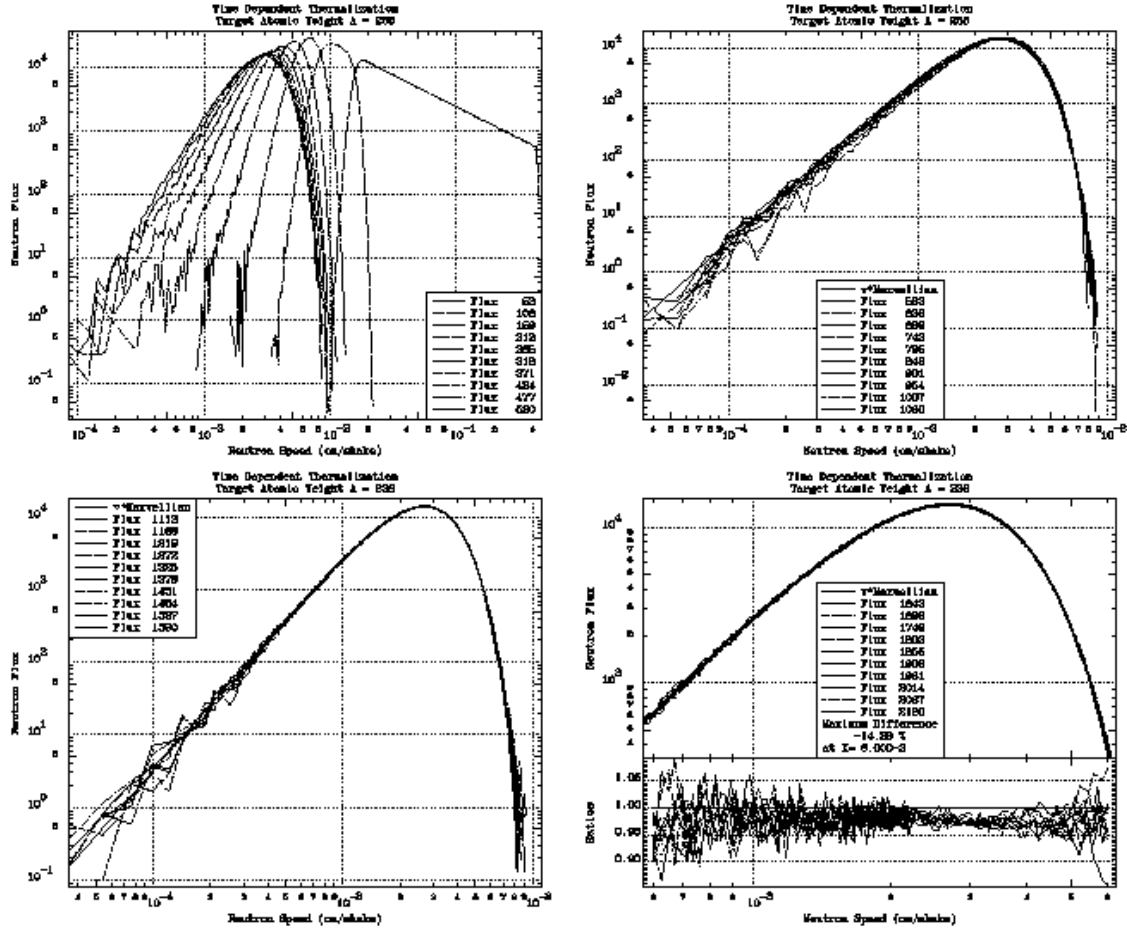


Figure 7: Time dependent thermalization without absorption; atomic weight = 238

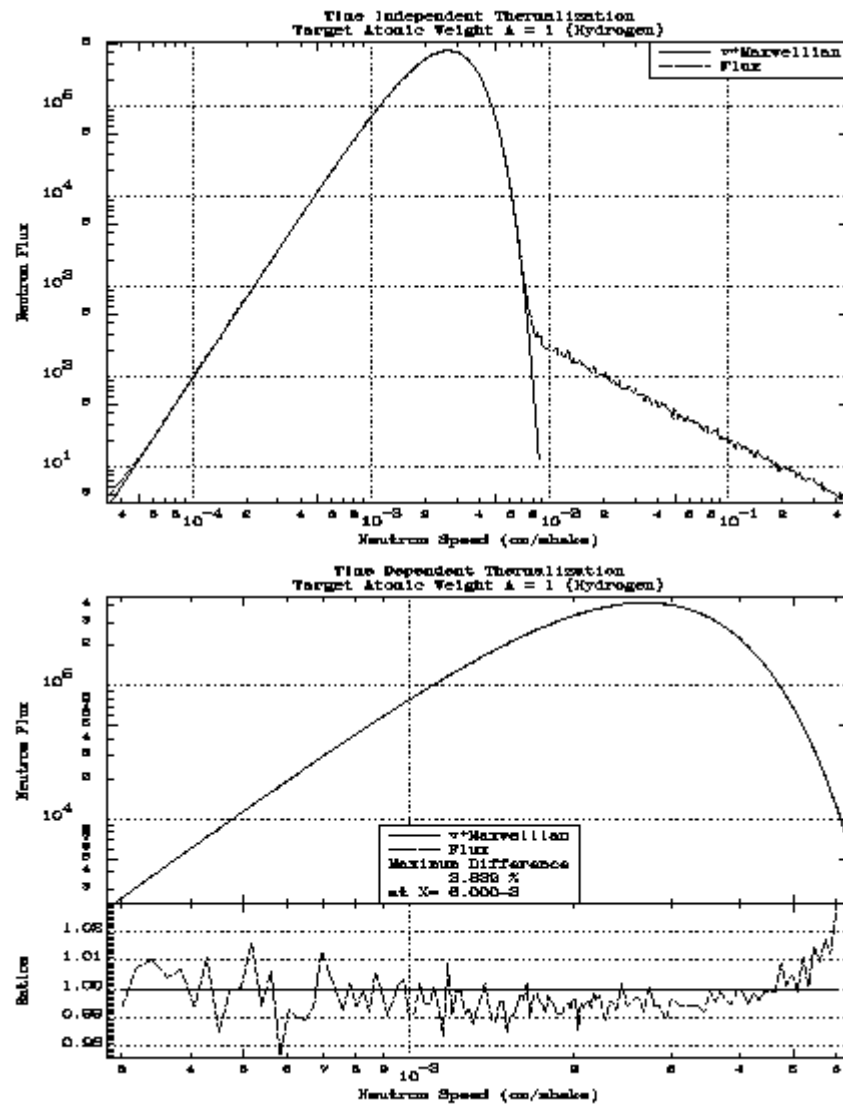


Figure 8: Time independent thermalization with absorption; atomic weight = 1

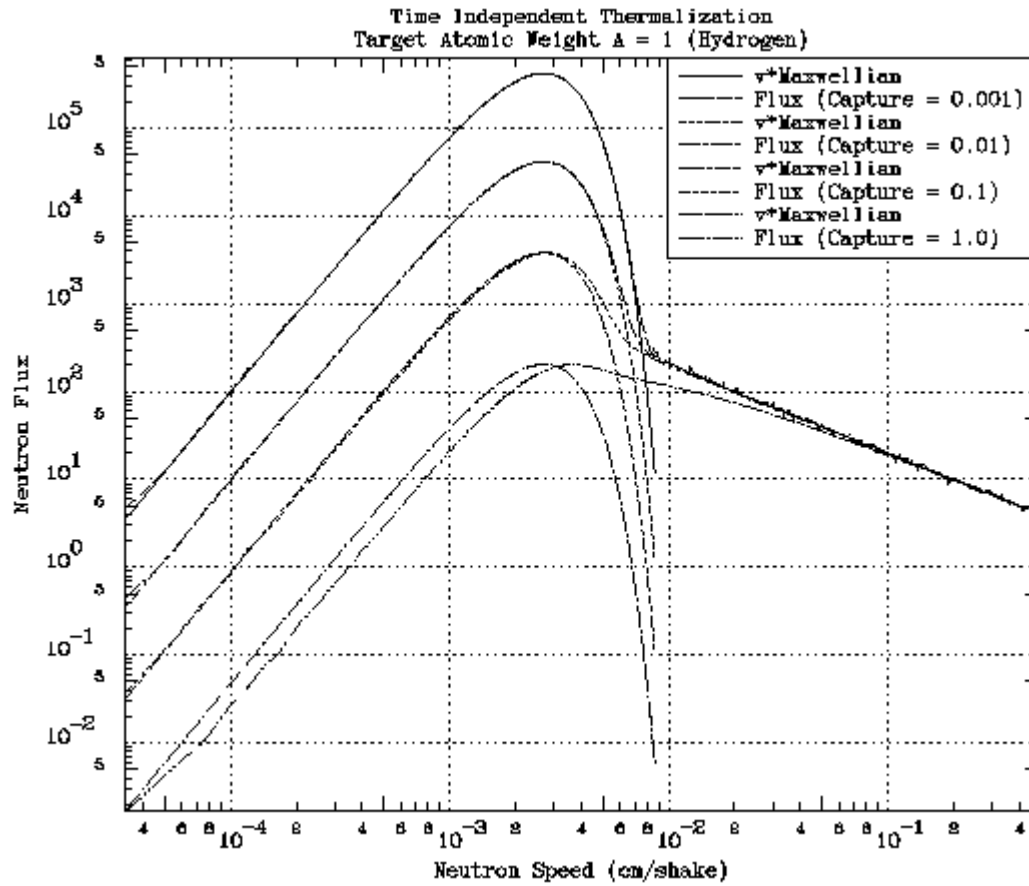


Figure 9: Time independent thermalization with absorption; atomic weight = 1

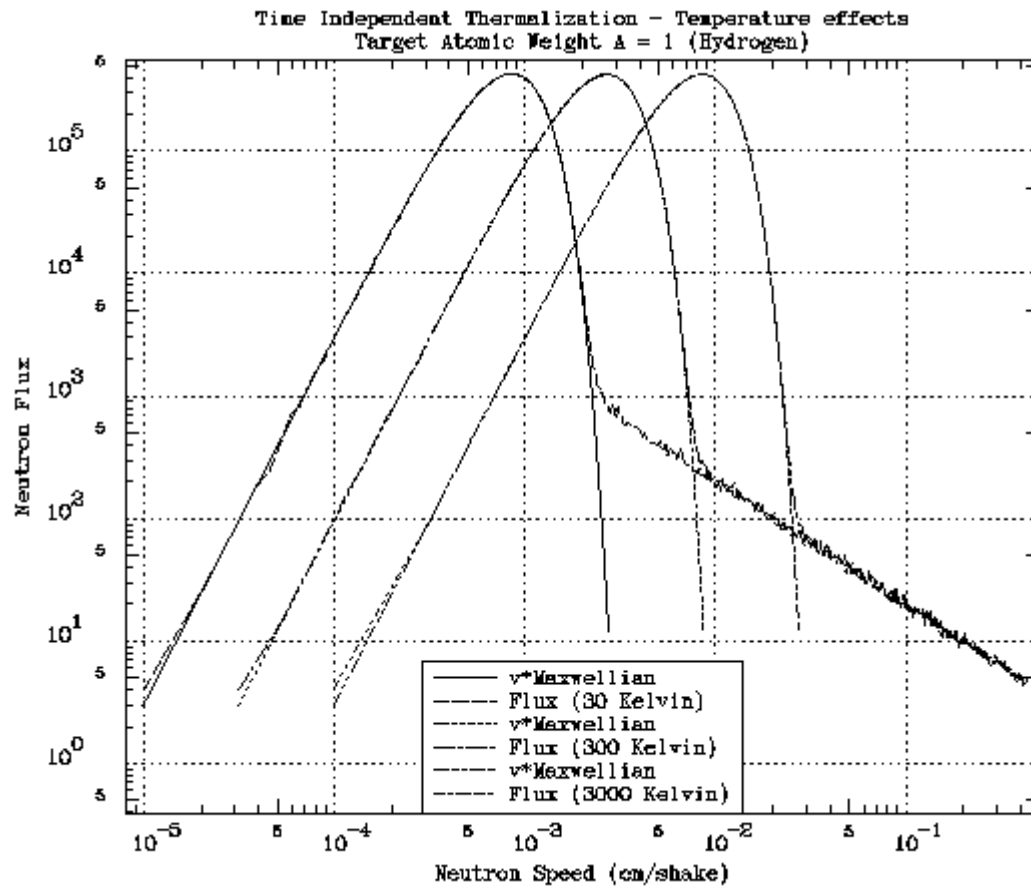


Figure 10: Time independent thermalization without resonance; atomic weight = 1

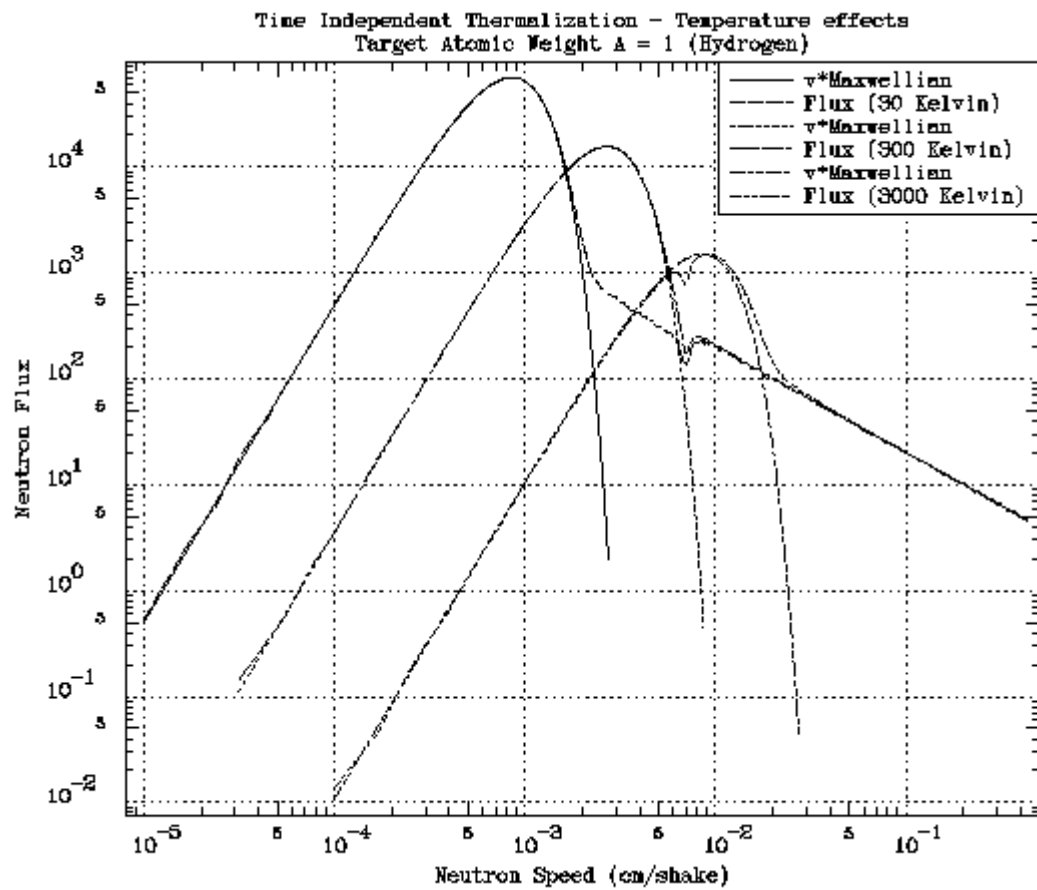


Figure 11: Time independent thermalization with resonance; atomic weight = 1

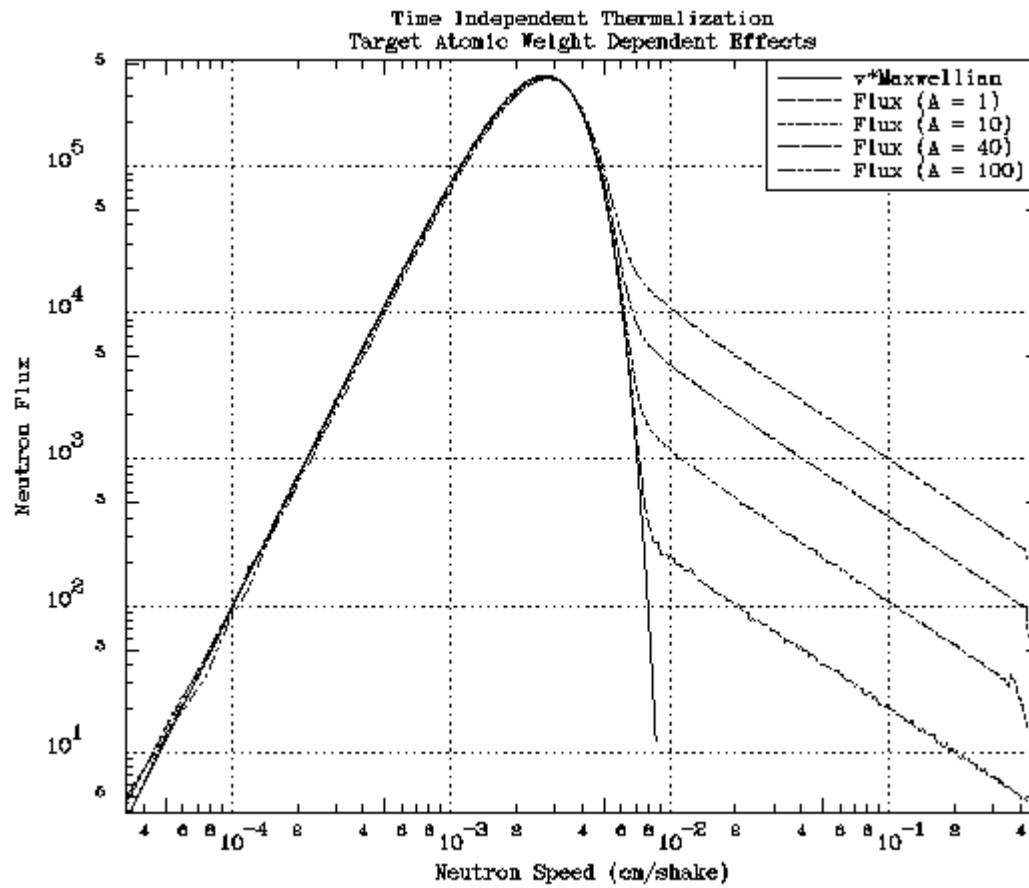


Figure 12: Time independent thermalization without resonance

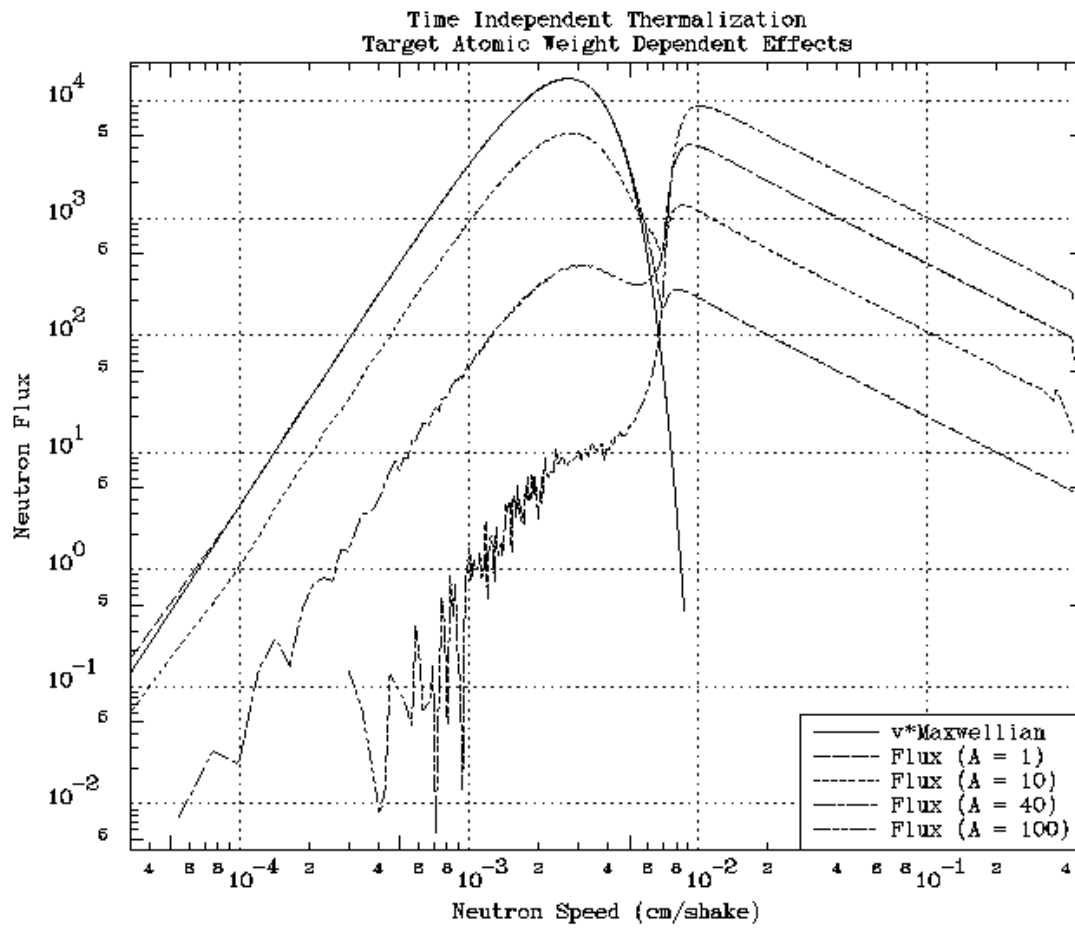


Figure 13: Time independent thermalization with resonance